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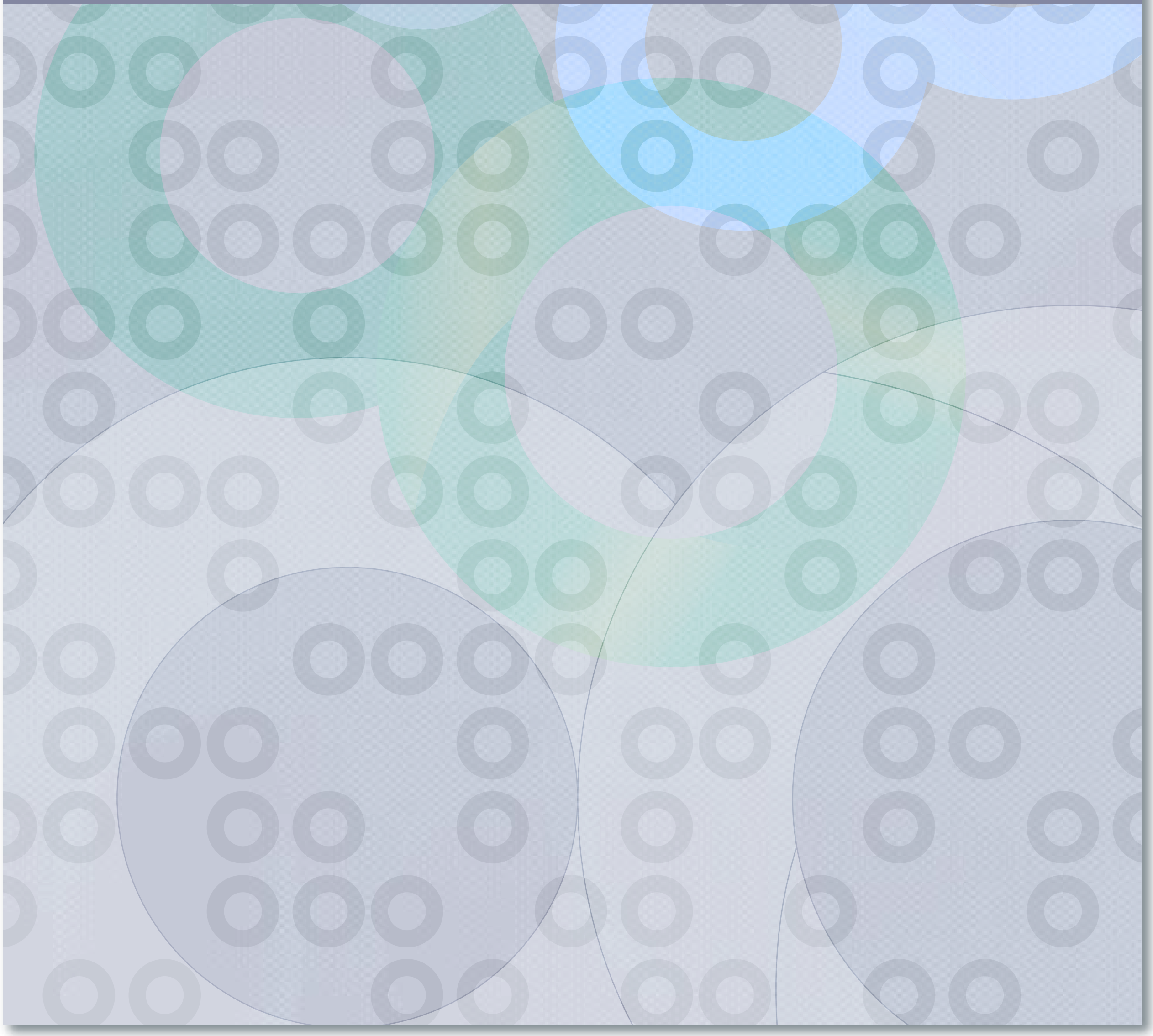
International Project Research-Workshop (I)

Advancing Materials Data, Design and Discovery

Editors: Kulbir Ghuman, Pierluigi Cesana, Kenji Kajiwara, Yu Kaneko,
Linh Thi Hoai Nguyen, Daniel Packwood,
Yasser Salah Eddine Bouchareb, Aleksandar Staykov

九州大学マス·フォア·インダストリ研究所



MI Lecture Note Vol.103 : Kyushu University

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About MI Lecture Note Series

The Math-for-Industry (MI) Lecture Note Series is the successor to the COE Lecture Notes, which were published for the 21st COE Program "Development of Dynamic Mathematics with High Functionality," sponsored by Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT) from 2003 to 2007. The MI Lecture Note Series has published the notes of lectures organized under the following two programs: "Training Program for Ph.D. and New Master's Degree in Mathematics as Required by Industry," adopted as a Support Program for Improving Graduate School Education by MEXT from 2007 to 2009; and "Education-and-Research Hub for Mathematics-for-Industry," adopted as a Global COE Program by MEXT from 2008 to 2012.

In accordance with the establishment of the Institute of Mathematics for Industry (IMI) in April 2011 and the authorization of IMI's Joint Research Center for Advanced and Fundamental Mathematics-for-Industry as a MEXT Joint Usage / Research Center in April 2013, hereafter the MI Lecture Notes Series will publish lecture notes and proceedings by worldwide researchers of MI to contribute to the development of MI.

October 2022
Kenji Kajiwara
Director, Institute of Mathematics for Industry

Advancing Materials Data, Design and Discovery

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Preface

This lecture note is a collection of extended abstracts presented at the symposium "Advancing Materials Data, Design, & Discovery" held at *I2CNER Hall C, Ito Campus, Kyushu University*, from April 23–25, 2025.

The symposium was organized and hosted by the International Institute for Carbon-Neutral Energy Research (I2CNER), the Institute of Mathematics for Industry (IMI), Kyushu University, and the Computational Energy Materials Design Infrastructure (CEMDI) platform at INRS.

This event was supported by the FY2025 IMI Joint Usage International Project Research-Workshop (I): *"Promoting Materials Data, Design, and Discovery"* (Reference No: 2025B007).

Artificial Intelligence (AI) is transforming Materials Science, with Machine Learning enabling data-driven predictions, accelerated discoveries, and the integration of informatics-based approaches alongside traditional computational methods. The application of AI in this field relies on novel methodologies that combine insights from both materials science and information technology, fostering a close synergy between disciplines. International efforts—including initiatives in the U.S., Europe, China, and Japan—have advanced the development of AI-based tools for materials discovery, with collaborations between academia and industry playing a key role in driving progress.

The 2025 symposium brought together computational and experimental materials scientists, as well as mathematicians, to discuss breakthroughs in AI-driven materials research. Topics included the integration of computational chemistry and physics methods, emerging computational techniques, the generation and use of high-quality datasets, and new mathematical models for complex materials systems. Collaborative initiatives between Japan and Canada, supported by research hubs and joint programs, highlighted the global and interdisciplinary nature of this work.

This symposium marked the fourth edition of the series overall (and the third with participation from CEMDI), which was launched in 2022 under the framework of the IMI Joint Usage Research Programs. Over the years, the series expanded internationally, fostering exchange, networking, and collaboration among researchers from multiple countries. We hope that the discussions and findings presented in this volume will continue to inspire innovation and strengthen international partnerships in AI-driven materials science.

The Organizers

Kulbir Ghuman

Pierluigi Cesana

Kenji Kajiwara

Yu Kaneko

Linh Thi Hoai Nguyen

Daniel Packwood

Yasser Salah Eddine Bouchareb

Aleksandar Staykov

Program

3rd CEMDI-PAIMS SYMPOSIUM
ADVANCING MATERIALS DATA, DESIGN, & DISCOVERY

Hosted by:
International Institute for Carbon-Neutral Energy Research (I2CNER)
Institute of Mathematics for Industry (IMI)
Kyushu University, Japan

Date: April 23–25, 2025
Venue: I2CNER Hall C, Ito Campus, Kyushu University

WEDNESDAY, APRIL 23, 2025

Time: 9:30 AM – 5:20 PM (JST)

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** — Rusoma Akilimali (Technology and Innovation Advisor, PRIMA, QC, Canada)
  Promoting Québec-Japan Collaboration in Advanced Materials

- **10:00 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
- **10:10 AM** — Kulbir Ghuman (Director CEMDI, Associate Professor, INRS, Université du Québec, Canada)
  Computational Energy Materials Design Infrastructure (CEMDI): Goals and Opportunities
- **10:20 AM** — Aleksandar Staykov (Associate Professor, I2CNER)
  Perspective of Artificial Intelligence in Materials Science (PAIMS)

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, Canada)
  Machine Learning Assisted Design of Porous Materials for CO2 capture using Integrated Atomistic Scale and Process Scale simulations
- **11:40 AM** — Daniel Packwood (Associate Professor, iCeMS, Kyoto University, Japan)
  Machine learning for functional molecular materials and supramolecular assemblies

12:10 PM – 1:10 PM — Lunch

Session III: AI for Materials Discovery

Chair: Tsuneyuki Ozaki

- **1:10 PM** — Adroit Fajar (Assistant Professor, I2CNER, Kyushu University)
  Can AI Truly Revolutionize Molecular Design?
- **1:40 PM** — Adrian Xiao Bin Yong (Postdoctoral Fellow, I2CNER CESD, Kyushu University)
  Dismai-Bench: Benchmarking generative models using disordered materials
- **2:10 PM** — El Tayeb Bentria (Researcher, QEERI, HBKU, Qatar)
  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 H2S 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

THURSDAY, APRIL 24, 2025

Time: 9:30 AM – 5:00 PM (JST)

Session I: Computational Chemistry for Material Design

Chair: Chandra V. Singh

- **9:30 AM** — Gilles Peslherbe (Professor, Concordia University, 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)
  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 SrTiO3

10:50 – 11:00 AM — Coffee Break

Session II: AI for Materials Discovery

Chair: Sergei Manzhos

- **11:00 AM** — Kazuki Yoshizoe (Professor, RIIIT, Kyushu University)
  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)
  Accelerated discovery of novel proton conducting ceramics utilizing experimental data and machine learning

12:20 – 1:20 PM — Lunch

Session III: Modeling and Calculations: From Atomic Structure to Applications

Chair: Edoardo Fabbrini

- **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** — Shunsuke Kobayashi (Assistant Professor, Osaka University, Japan)
  Dislocation and Disclination in Crystalline Materials: A Differential Geometry Approach
- **2:20 PM** — Fiorenzo Vetrone (Professor, INRS, Université du Québec, Canada)
  Frontiers in Rare Earth Doped Nanoparticles: Design, Properties, and Applications

2:50 – 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)
  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

FRIDAY, APRIL 25, 2025

Time: 9:30 AM – 5:30 PM (JST)

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** — Sergei Manzhos (Associate Professor, Institute of Science Tokyo)
  Large-scale electronic structure materials modeling with the help of machine learning-enhanced DFTB and OF-DFT
- **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

Session II: Materials Discovery for CO_2 Capture – Experiments, Computational Chemistry & AI

Chair: Linh T. H. Nguyen

- **11:30 AM** — Paul O'Brien (Associate Professor, York University, Canada)
  Machine Learning for Direct Air Carbon Capture: Challenges and Opportunities
- **12:00 PM** — Tanay Sahu (PhD Student, York University, Canada)
  Identification and Evaluation of CO_2 Photocapture Materials
- **12:20 PM** — Victor Eke (Master's Student, York University)
  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
- **12:40 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 – 2:00 PM — Lunch (Lunch Meeting with Directors – *By Invitation Only*)

Session III: Modeling and Calculations – From Atomic Structure to Applications

Chair: Jacqueline Hidalgo-Jiménez

- **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)
  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, Délégation générale du Québec à Tokyo, Japan)
  Quebec-Japan Collaboration
- **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** — Oral Presentation Awards (Sponsored by Royal Society of Chemistry)

- **5:00 PM** — Organizers' Closing Remarks
- **5:15 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)

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Tatsumi Ishihara（International Institute for Carbon-Neutral Energy Research, Kyushu University, Fukuoka, Japan ; Department of Automotive Science, Kyushu University, Fukuoka, Japan）
Kaveh Edalati（International Institute for Carbon-Neutral Energy Research, Kyushu University, Fukuoka, Japan ; Department of Automotive Science, Kyushu University, Fukuoka, Japan）

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Promoting Québec-Japan Collaboration in Advanced Materials

Rusoma Akilimali

Advanced Materials Research and Innovation hub, Montreal,
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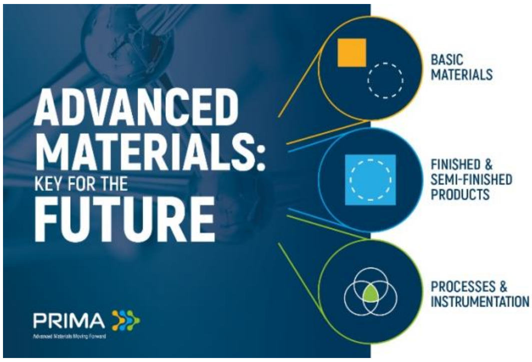

PRIMA Québec, the Advanced Materials Research and Innovation hub, supports and facilitates the advanced materials ecosystem by promoting collaborative innovation for the economic development of Quebec. It is the privileged catalyst between the industrial and research communities, and has nearly 170 industrial members, for a total of 220 members. Among 181 funded projects between 2015 and 2024, about a hundred intellectual properties have been generated.

Mandate

- Support Québec's industrial and societal challenges by stimulating collaborative innovations between industries and researchers in the advanced materials sector
- Facilitate access and increase support for leading-edge equipment users, while providing the expertise required for innovation projects
- Ensure the transfer of knowledge by training and preserving the qualified personnel currently working within researcher-industry partnerships

PRIMA is a leader in advanced materials through its knowledge of the ecosystem and its expertise when supporting companies – for a more competitive Québec in a number of areas thanks to sustained growth in the advanced materials ecosystem. An advanced material can be defined as any new or significantly improved material that provides a distinct advantage in (physical or functional) performance when compared to conventional materials. As a Sectoral Industrial Research Group (SIRG), PRIMA Québec relies on financial support from both the Quebec government and the private sector when promoting research-industry relations.

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

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Abstract: The Computational Energy Materials Design Infrastructure (CEMDI), www.cemdi.inrs.ca, founded in 2022 at INRS-EMT, drives innovation in clean energy through advanced computational research and global collaboration. By leveraging Quebec's leading computational expertise, CEMDI fosters national and international partnerships to tackle climate change challenges. With established collaborations in Japan, we are actively expanding our network to accelerate breakthroughs in sustainable materials research.

This talk will outline CEMDI's key objectives: driving energy and materials innovation, facilitating global collaborations, empowering emerging researchers, bridging the academia-industry gap, and advancing equity, diversity, and inclusion in materials science. I will also draw on examples from my own research to illustrate how CEMDI's approach translates into tangible advancements in energy materials design. Additionally, I will highlight CEMDI's ongoing initiatives, interdisciplinary events that unite researchers from mathematics, chemistry, physics, materials science, engineering, and AI, as well as collaboration opportunities for students, principal investigators, and industry partners within CEMDI's ecosystem - all aimed at accelerating sustainable technology development to combat climate change.

About the speaker: Kulbir Kaur Ghuman, PhD is an early-career researcher, appointed as Associate Professor at Institut national de la recherche scientifique, Centre Énergie Matériaux Télécommunications (INRS-EMT) and a Tier-2 Canada Research Chair in 'Computational Materials Design for Energy and Environmental Applications'. Before joining INRS-EMT she worked as a postdoctoral fellow at University of Toronto, Paul Scherrer institute (Switzerland), and Kyushu University, (Japan). Her current laboratory, Insilico Matters Laboratory (IML), is equipped with advanced software and computational infrastructure, dedicated to understanding the theoretical underpinnings of the behavior of complex materials and chemical reactions. She has established several novel structure-property relationships and mechanisms for optimizing fuel cell materials and designing efficient catalysts imperative for mitigating climate change. Currently, she is also spearheading a recently established consortium 'Computational Energy Materials Design Infrastructure (CEMDI)' at INRS that aspires to foster innovation in the area of energy materials research via collaboration and advanced computational techniques.

Self-supervised probabilistic models for exploring shape memory alloys

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Recent breakthroughs in machine learning (ML) are transforming the landscape of high-performance materials design, yet developing robust models to unravel complex structure-property relationships remains a significant challenge. This difficulty is exacerbated by the scarcity of labeled datasets with well-characterized crystal structures, particularly for materials where functional properties are tightly linked to crystallographic symmetry. In this work, we present a self-supervised probabilistic model (SSPM) that autonomously learns unbiased atomic representations from crystal structure data derived from high-throughput first-principles calculations. By leveraging these representations, SSPM effectively uncovers the probabilistic relationships between material composition and crystal structure, significantly enhancing the performance of downstream ML models. To demonstrate the model's potential, we apply SSPM to the discovery of shape memory alloys (SMAs). Out of the top 50 predictions made by the model, 23 have been experimentally or theoretically confirmed as SMAs, including the identification of a novel SMA candidate, MgAu. This approach not only advances materials discovery but also offers a powerful tool for accelerating the design of functional materials.

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

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Metal organic frameworks (MOFs) are crystalline, nanoporous materials that have attracted significant attention as sorbents for gas separation applications such as CO_2 capture, where they are being commercialized. While there are now many studies that use computational high-throughput (HT) screening and machine learning models to accelerate the screening of MOFs CO_2 capture, almost all screen the materials for a select few adsorption properties, such as CO_2 capacity or selectivity. Very few studies consider the industrial process that the materials will be used in. In this work, atomistic scale modeling is integrated with detailed process level simulations to evaluate how a material will perform in a real gas separation process. This allows us to evaluate MOFs based on more holistic metrics such as the energy consumption of the CO_2 capture, or to determine how much MOF sorbent would be required. Machine learning models have been used to accelerate various stages of this multi-scale workflow. This has allowed us to screen more than ~30,000 experimentally characterized MOFs in a month, whereas the screening only 2,000 MOFs without the ML acceleration previously took close to a year. The goal of this work is to design materials at the atomic level, that will be high performing based on industrial scale metrics such as how much energy the process will use or how pure the CO_2 that is extracted will be.

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Machine learning for functional molecular materials and supramolecular assemblies

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Over the last several years, machine learning and other data science techniques have made a profound impact on computational materials science. On the one hand, data science techniques have significantly broadened the scope of molecular simulation, allowing us to study more complex materials over longer time scales. On the other, these techniques have allowed us to extract obscure structure-function correlations from material databases, which can subsequently be used to design new functional materials. In this presentation, I will illustrate these points by introducing two topics from our group's research. The first topic concerns the formation of supramolecular clusters *via* on-surface molecular self-assembly (Figure 1). By utilizing machine-learned intermolecular potentials, we have developed new methodology for simulating the molecular self-assembly process and predicting what kinds of supramolecular clusters will form. This simulation enables one to screen different types of molecules for the purposes of designing new supramolecular materials with novel functionality [1]. The second topic concerns the design of organic semiconductor materials. We have developed a pipeline which integrates both supervised and unsupervised machine learning, as well as chemical expertise, for discovering organic semiconducting materials with specific band gaps and high charge mobilities [2,3].

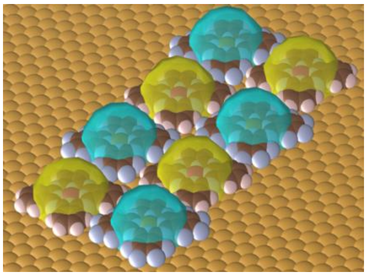

Figure 1. Simulated assembly of phthalocyanine molecules on a gold surface.

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Can AI Truly Revolutionize Molecular Design?

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Artificial intelligence (AI) has been hailed as a game-changer across nearly every scientific discipline, and chemistry is no exception. With the promise of accelerating molecular discovery, predicting novel compounds, and optimizing reaction conditions, AI-driven approaches have captured the imagination of researchers and industry leaders alike. But amidst the excitement, a fundamental question remains: Can AI truly revolutionize molecular design, or is it just another overhyped tool? [1] In this talk, we'll explore the real impact of AI on molecular design from the perspective of an experimental chemist engaged in various data science projects.

Before discussing AI's role, it is important to understand the conventional approach to molecular design. In our research group, we developed a novel chemical—an ionic liquid (IL) for metal separation—aimed at improving processes in the metal mining industry [2]. After synthesizing the IL, we further optimized it by transforming it into a membrane for real-world industrial applications [3,4]. However, achieving a practical solution required optimizing numerous experimental parameters, a painstaking process that spanned several years. Eventually, we succeeded in developing a useful technology for industry [5], but the process underscored the challenges of traditional molecular design: it is slow, labor-intensive, and heavily reliant on trial and error.

Recognizing the potential of machine learning (ML) to accelerate molecular discovery—even before the advent of models like ChatGPT—we expanded our approach. Instead of designing a single novel chemical at a time, we generated a library of over 100 candidate ILs and used ML to screen for the most promising ones based on their metal selectivity. Despite working with relatively small datasets, we leveraged precise molecular descriptors (such as the σ-profile) and a simple yet effective ML model—random forest—to achieve reasonably accurate predictions. Following ML-based predictions, we successfully synthesized and tested three ILs that demonstrated selective extraction capabilities for critical metals such as platinum (Pt), lithium (Li), and neodymium (Nd) [6]. Encouraged by these results, we extended our exploration to deep eutectic solvents (DESs), a new class of green extractants considered potential successors to ILs. However, because DESs are a relatively new material, relevant datasets were virtually nonexistent. To overcome this, we integrated ML predictions (random forest, extreme gradient boosting, and multilayer perceptron) with thermodynamic principles governing eutectic mixtures. This combined approach allowed us to estimate the formation of approximately 3,000 DESs with reasonable accuracy [7].

More recently, we have turned our attention to generative AI, which offers the potential to facilitate inverse molecular design—where desirable properties dictate molecular structures rather than vice versa. Generative models, such as variational autoencoders (VAEs) and generative adversarial networks (GANs), can explore vast chemical spaces to identify promising IL candidates. However, these models typically require extensive datasets, and the availability of IL-related data is limited. To address this challenge, we fine-tuned a large language model (LLM), specifically GPT [8], on a small IL dataset to generate novel IL structures. As shown in Figure 1(a), the model achieved a low test loss (approximately 0.1), indicating its ability to learn chemical grammar patterns from the dataset and reliably generate new ILs. These generated molecules were further optimized for specific properties—such as CO_2 dissolution and eco-friendliness—using the SMILES-X molecular property prediction tool [9]. To validate our results, we cross-checked them with density functional theory (DFT) and COSMO-RS simulations, followed by surrogate experimental measurements [10].

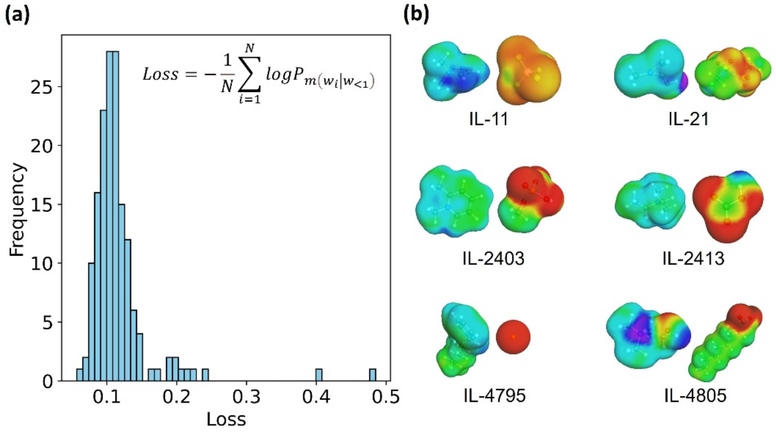

Figure 1. (a) Test loss distribution and (b) a few examples of the generated ILs.

AI is already demonstrating its ability to transform molecular design by significantly accelerating discovery and optimization processes. While traditional methods remain crucial, AI-driven approaches are enabling researchers to explore chemical spaces at unprecedented speeds. However, challenges such as limited datasets and the need for experimental validation still remain. As AI techniques continue to evolve, their integration with experimental chemistry will likely unlock even greater advancements in materials and molecular design.

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Advancing Materials Data, Design, and Discovery

April 2325, 2025, Kyushu University, Fukuoka, Japan

Dismai-Bench: Benchmarking generative models using disordered materials

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(joint work with Tianyu Su and Elif Ertekin)

Generative modeling of material structures has received significant attention in recent years, with the main interest of leveraging them for materials discovery [1, 2]. Initially limited to the generation of molecules [3, 4] and proteins [5], generative modeling has since advanced to include inorganic materials [6, 7, 8] as well. However, current efforts for inorganic materials [12, 13, 14] have predominantly focused on small, periodic crystals ($\leq$20 atoms), and there has been less emphasis on disordered systems, despite their relevance across a wide spectrum of applications [9, 10, 11]. Disordered systems usually have complex and irregular structures, necessitating large atomic representations and requiring more powerful generative models than those developed for simple crystals. Furthermore, current generative models have also been developed by evaluating on the new unverified materials being generated, using heuristic metrics such as charge neutrality, leading to a narrow evaluation of the models' performance. It is therefore difficult to make meaningful comparisons between model architectures, and determine which design choices are better. To develop better generative models, for both the generation of simple crystals and more complex disordered structures, better evaluation methods are needed.

In this work, we present the Disordered Materials & Interfaces Benchmark (Dismai-Bench) [15], a new framework for evaluating generative models of inorganic materials. Dismai-Bench evaluates models using datasets of disordered structures with a wide range of disorder, as shown in Fig. 1. Models are trained on one dataset at a time, and evaluated through direct comparison between the generated structures and the training structures using structure similarity metrics. By restricting the material space of generated materials, this approach circumvents the issues of existing methods which attempt to evaluate on new unknown materials being generated. The Dismai-Bench datasets were also chosen such that they are sufficiently challenging to provide meaningful evaluation of a model's performance. Dismai-Bench assesses a generative model's capability to learn complex structural patterns, and informs model architecture design whether for the generation of small crystals or large disordered structures.

We selected four recent diffusion models to be benchmarked on Dismai-Bench, including two models that use graph representations (CDVAE [12] & DiffCSP [13]) and two

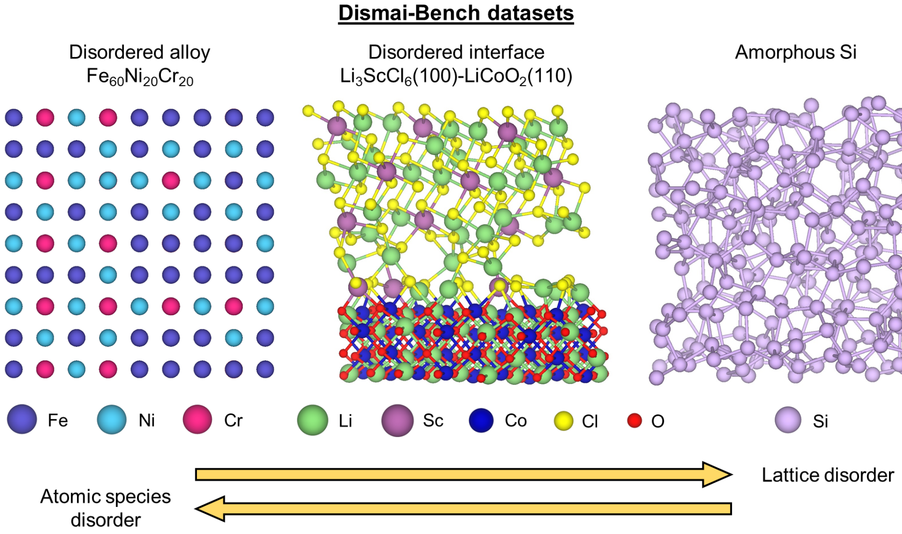

FIGURE 1. Datasets used in Dismai-Bench. Figure reprinted with permission from [15].

models that use coordinate-based representations (CrysTens [16] & UniMat [14]). The coordinate-based models use simple material representations derived from raw atomic coordinates as input to the generative models. On the other hand, the graph representations contain atom neighbor information, more comprehensive geometrical features, and symmetry invariances, providing stronger expressive power than the coordinate-based representations. We also included a generative adversarial network (GAN) that we developed, known as CryinGAN [15], in the benchmark results. CryinGAN is a model that we designed to demonstrate the application of Dismai-Bench in the development of a generative model. We chose a simple coordinate-based representation, and tested multiple different GAN architectures. Through direct comparison between the generated and training structures, we were able to identify the best performing architecture (CryinGAN), as well as reasons for why the other architectures were less successful. We use CryinGAN to demonstrate the benefits and importance of robust generative model evaluation.

An overall ranking of all generative models based on their general performance on each Dismai-Bench dataset is shown in Fig. 2 (refer to [15] for full details of the benchmark results). The graph diffusion models, CDVAE and DiffCSP, demonstrated the best performance overall due to the strong expressive power of the graph representation. However, the graph models were only successful in performing diffusion on atomic coordinates alone, but suffered when performing joint diffusion with atomic species or lattice parameters, indicating room for further improvement. On the other hand, the

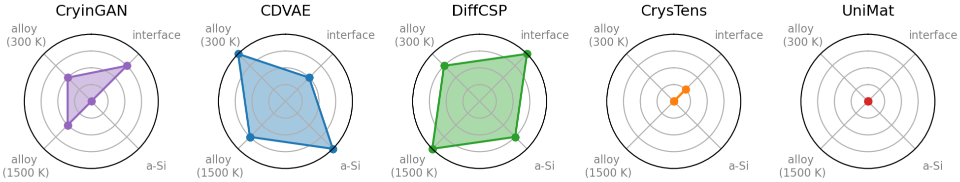

Figure 2. Spider chart of generative model ranking based the models' general performance on each dataset. The models are ranked 1-5, where the outermost ring corresponds to rank 1 (best), and the center of the chart corresponds to rank 5 (worst). Figure reprinted with permission from [15].

coordinate-based diffusion models, CrysTens and UniMat, struggled with most tasks in Dismai-Bench. These models were adapted from generative models used for image and video generation, and the benchmark results show that such models do not translate well to learning complex atomic structures. The less expressive coordinate-based representation also contributed to these models' weaker performance. For CryinGAN, despite that it also used a coordinate-based representation, it was able to demonstrate superior performance to the coordinate-based diffusion models, even though diffusion models are often reported to outperform GANs in image synthesis tasks [16, 17, 18]. However, CryinGAN does not outperform the graph diffusion models, likely as a result of its weaker expressive power and lack of invariances. Nonetheless, CryinGANs surprisingly good performance is a testament to the importance of robust evaluation in model development.

In summary, we have developed the first vigorous benchmark for generative models of inorganic materials that provides meaningful evaluation for comparing between architectures, understanding model strengths and weaknesses, and ultimately informing design choices. Building the next generation of generative models will rely on not only developing better architectures and representations, but also adopting better evaluation methods. We hope that this work will help advance future generative models for both ordered and disordered materials, and inspire the development of other new innovative benchmarks.

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

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Large Language Models (LLMs) are fundamentally next-word prediction systems trained on massive text corpora, yet they offer capabilities that extend well beyond language generation. Recent research papers demonstrate how they can be immensely beneficial in computational materials science, making it imperative to expand our horizons and explore this new territory. This paper discusses recent research in computational materials science, using examples to illustrate the role of large language models (LLMs) in the field. The examples will include: First, a case where their integration has facilitated progress, where we highlight how LLMs~~,~~ when integrated into domain-specific frameworks, have accelerated problem-solving in materials science such as autonomous LLM-based "agents" capable of independently performing and refining computational tasks. Second, we present our in-house tool *Kateeb* where LLMs offer comprehensive, end-to-end solutions through automated database generation and the structuring of large datasets. Third, we present our research on understanding carbonyl corrosion reaction mechanisms, a challenge that is beyond the capabilities of LLMs and explain why.

1. Introduction

The integration of Large Language Models (LLMs) into scientific research has opened new horizons for knowledge discovery and innovation. In materials science, researchers have begun leveraging LLMs for tasks ranging from automated literature reviews to text-guided experimental design, thereby accelerating research workflows while reducing human effort and time expenditures [1]. Recent progress in LLM architecture has revealed not only their ability to parse vast datasets rapidly but also their capacity to generate structured outputs, from experiment notebooks computational input files from different codes and research papers, at scales traditionally unattainable by human experts alone [2].

Historically, materials science has evolved through distinct paradigms, from the discovery of natural materials and development of standardized processing techniques for agricultural use, to the industrial revolution, and modern design of methodologies that have each required higher-level data management and interpretation [3], [4], [5]. Today's "fourth industrial revolution," driven by artificial intelligence (AI) and automation, has stimulated research in "intelligent materials" and sustainability-focused manufacturing for example However, the vast amount of data generated in the last 200 years, encompassing millions of material structures, makes it impossible for the human brain to reason alone and identify the next major breakthrough. LLMs has emerged as powerful tools: they can parse extensive repositories of text-based documents, extract and compile relevant information, and deliver it in readily usable formats [2]. Such an approach has demonstrated orders-of-magnitude speed improvements processing one paper in mere seconds compared to tens of minutes or hours by a human expert [6].

Despite these advantages, several questions remain regarding the scope and limitations of

LLMs in computational materials science. Complex atomistic problems, especially those involving multiple quantum mechanical interactions and chemical reaction pathways in catalysis and corrosion science, are not trivially distilled into purely language-based descriptions. For instance, iron carbonyl ($Fe(CO)_x$, x=1-5) corrosion serves as an example of a phenomenon whose mechanistic intricacies challenge the use of LLM approach to speed up the tasks [7].

This work aims to illuminate the broader landscape of LLM integration into computational materials science by: (i) discussing core advantages and disadvantages of adopting these models in research workflows, (ii) presenting practical cases where LLMs have already accelerated materials discovery and design, (iii) detailing a specific scientific challenge catalytic reactions that remains beyond the direct capabilities of current LLMs.

2. Advantages and Disadvantages of Large Language Models in Materials Science

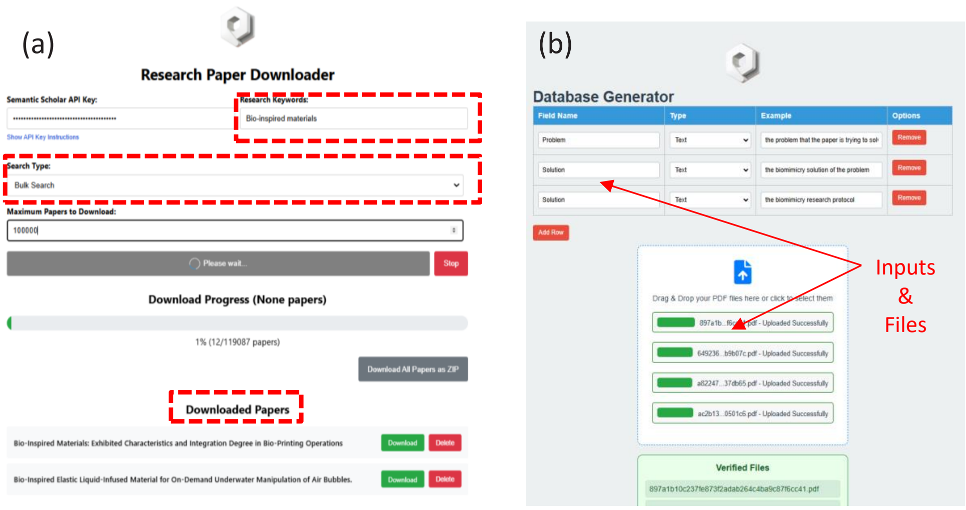
Large Language Models (LLMs) have gained prominence for their remarkable ability to process natural language at an unprecedented scale. This aptitude has immediate benefits for the materials science community, particularly when handling large volumes of unstructured text data such as journal articles, lab reports, and simulation logs. One of the primary advantages of LLMs lies in their capacity for rapid data mining and synthesis[8]. By extracting key parameters such as processing temperatures, materials compositions, and performance metrics from heterogeneous sources, LLMs can quickly transform unstructured data into structured, easily searchable databases. This streamlined approach not only accelerates literature reviews but also aids in the identification of emerging research trends, guiding investigators toward promising new materials or unexplored processing methods [1], [8]

In addition to accelerating data management, LLMs have begun to integrate with computational toolchains. Newly emerging "agent" paradigms extend beyond passive text generation, facilitating tasks such as writing simulation input scripts or specifying experimental conditions in real-time[9]. These integrated systems can greatly reduce the knowledge gap between specialists in machine learning and those in computational materials science, thereby democratizing access to advanced analytical workflows.

Despite these advantages, LLMs also face limitations that restrict their utility in certain contexts. For instance, while they excel at parsing existing data and generating high-level summaries, they often lack intrinsic understanding of fundamental physical principles. As a result, purely language-based models can struggle with understanding complex atomistic phenomena especially if the prompt commands are not engineered correctly. leading to incomplete or even misleading conclusions if not carefully supervised. Another concern centers on their reliance on preexisting datasets and potential bias in training corpora, which can diminish the reliability of their predictions in less-studied domains or novel material systems.

3. Case Studies of LLM-Driven Acceleration in Materials Research

Multiple case studies highlight how integrating LLMs into computational workflows can substantially accelerate materials research and discovery [1]. One case study involves structured data generation from vast corpora of scientific documents. As the volume of materials science publications grows exponentially, traditional manual curation often becomes prohibitively time-consuming and prone to human error. We have introduced an automated platforms named "Kateeb" [2] which is a specialized tool designed for scientists to efficiently download and compile large volumes of scientific literature focused on their specific research topics. By leveraging the advanced capabilities of GPT-4o, Kateeb enables researchers to construct accurate and reliable databases based on validated scientific findings. This platform ensures that the unstructured extracted data sourced from peer-reviewed publications, is converted to structured database to supporting rigorous meta-analyses, comprehensive trend assessments, and evidence-based research developments. These structured databases can be directly imported into statistical analysis toolkits or machine learning frameworks, enabling fast identification of trends such as the most effective synthesis routes for novel alloys or correlations between process conditions and material properties [1], [8]



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Bio-Inspired Elastic Liquid-Infused Material for On-Demand Underwater Manipulation of Air Bubbles.

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Figure 1: (a) Research paper downloader that can use scholar semantic API to download thousand of papers on selected topic selecting Bulk or relevant search, (b) Database generator that uses OpenAI API to read the PDF files and extract 100% structured data.

Finally, recent developments in “agenized” LLMs have demonstrated how natural language understanding can be fused with advanced simulation tools. These agents such as DARWIN 1.5 [9]autonomously generate computational input files for atomistic simulations (e.g., density functional theory or molecular dynamics), run those simulations, check the convergence of the results and interpret the results in real time [1], [9]. which promise to accelerate iterative design cycles in materials R&D. Although many of these tools are still in the experimental phase, preliminary evidence suggests they can dramatically reduce the time spent on routine tasks, freeing researchers to focus on conceptual breakthroughs and hypothesis-driven exploration.

3. A Scientific Challenge Beyond LLM Capabilities and Final Notes

While LLMs can rapidly analyze large volumes of text describing experimental observations and computational results, they face inherent limitations when it comes to explaining the fundamental physics and chemistry of a reaction, especially when there is no existing knowledge about it [10] . An example is carbonyl corrosion [7], where only one DFT study has calculated the adsorption and desorption energy of iron Pentacarbonyl on Iron surface, obtaining a value of about 3.8 eV. This value does not explain the phenomenon that occurs at temperatures between 100°C and 250°C.

Even if we assume an LLM could propose intricate reaction pathways similar to Figure 3, the complexity of the problem and the novelty of the catalytic reactions which lie beyond the scope of standard DFT, and the unlimited possiblites can lead to endless loop that the user have no say in it. As a result, a researcher who did not initiate this line of inquiry themselves would likely be unable to advance, since the necessary insights to progress would not be evident from the LLM’s output alone.

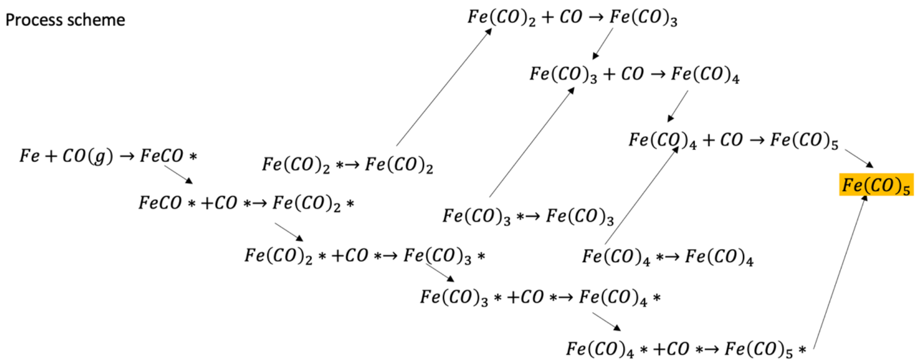

Figure 2: Schematic representation of pathways considered in this study leading to iron pentacarbonyl formation on Fe Surface.

Looking ahead, the continued evolution of LLMs in materials science will likely involve tighter integration with domain knowledge: ontology-driven data structures, specialized corpora, and direct incorporation of computational methods beyond language-based reasoning. As more sophisticated multi-modal AI approaches emerge, bridging text with computational physics, experimental data, and even real-time instrumentation control may become more feasible [6]. These developments could close some of the current gaps in understanding complex processes, paving the way for truly autonomous research systems.

5. Conclusion

Large Language Models (LLMs) are rapidly reshaping the research landscape in computational materials science, offering new horizon in knowledge extraction, database curation, and materials property prediction. Yet, their intrinsic constraints must be recognized to maintain scientific rigor. While LLMs excel at automating literature reviews, organizing extensive datasets, and highlighting emerging research trends, they lack the depth to independently formulate robust hypotheses or execute nuanced scientific writing.

In this work, we have shown how our tool, Kateeb, can efficiently download large amounts of data and use LLMs to extract information and generate structured databases. This process improves data management and speeds up research workflows. However, LLMs do not understand physical principles and cannot be used alone for material design, multi-scale modeling, or complex quantum mechanical problems such as carbonyl corrosion. To ensure reliable results, they must be combined with physics-based models and expert knowledge.

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

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Electrochemical energy conversion and storage are playing a key role in our transition to green energy future. Chemical reactions critical to this transition include CO2 reduction (CO2RR), nitrogen reduction reaction (NRR), hydrogen evolution reaction (HER), and oxygen evolution reaction (OER). Technologies facilitating these reactions require catalysts to accelerate chemical transformations of reactant species while maintaining stability – most of these catalysts utilize precious metals such as platinum and palladium. We need to design and optimize new catalytic materials made of less expensive materials or substantially decrease the utilization of expensive materials. However, the scaling relationships inherent in certain catalytic reactions present a technical challenge in achieving strong adsorption of some intermediates while maintaining weak adsorption of others, which leads to general activity-descriptor plots in a volcano plot, which limits the compositional space to few costly and non-earth abundant chemical elements. To overcome this barrier, we need catalysts comprising of earth-abundant chemical elements that circumvent such scaling relations. In this regard, high-entropy alloys (HEAs), typically composed of five or more equimolar elements, could provide unique opportunities to design catalysts that meet current state of the art catalyst but minimize or eliminate expensive elements since the cocktail effect offers promising opportunities to unlock remarkable properties.[1-4] However, the vast chemical space of HEAs make trail-and-error experimental approaches and even time-saving theoretical computation inefficient for HEA discovery. Moreover, for HEA catalysis, the structure-performance relations are unclear due to the complex surfaces.

Leveraging machine learning techniques to analyze local coordination environment of active sites, we have recently found that HEA catalysts are efficient to circumvent the scaling relationships in the hydrogen evolution reaction (HER) and CO_2 reduction reaction (CO_2RR), mainly due to diverse active sites on HEA surfaces, and thus breakthroughs in catalytic performance.[5, 6] Specifically, we found an unusual Sabatier principle on HEA surface and new descriptors of μ and σ in the Gaussian distribution [$X \sim N(\mu, \sigma^2)$] of ΔG_{H*} for HER activity on PtFeCoNiCu catalyst.[5] For CO_2RR, the rotation of key intermediate, *COOH and *CHO, on different surface sites of FeCoNiCuMo catalyst decreases the free energy change of the rate-determining step.[6] In addition, our ongoing investigations focus on elucidating the selectivity of C_{2+} products on HEA catalysts. In these HEA catalysis works, we have built a database of more than 10,000 adsorption energies of H, C, and O species on HEAs, and it is still growing. We believe that this database will significantly aid HEA catalyst researchers once integrated and made publicly accessible, and that the unique ability of HEA catalysts to circumvent the scaling relations could also lead to activity breakthrough in other reactions.

We will also present our recent data on computational catalyst design for other chemical reactions, including NRR and OER. Additionally, some results will be presented on the computational design of new materials for solid state batteries.

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

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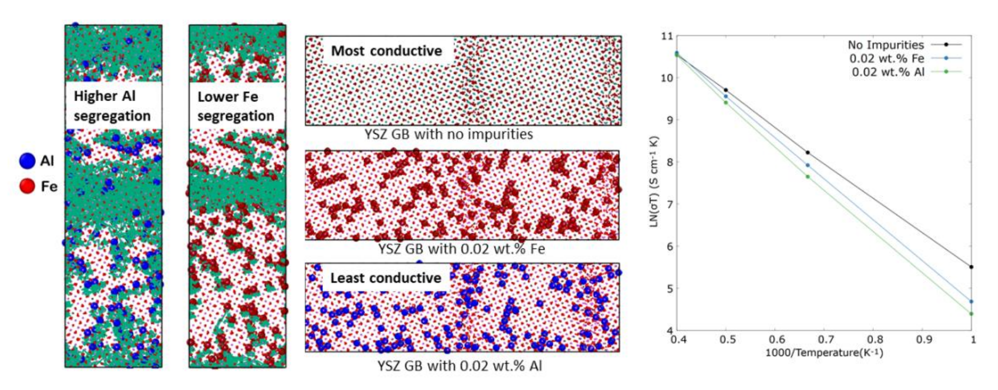
Yttria-stabilized zirconia (YSZ) is highly valued for its high ionic conductivity and thermal stability, making it indispensable in high-temperature applications like solid oxide fuel cells. However, performance in YSZ is intricately related to the behavior of impurities at grain boundaries, especially with respect to their effect on ionic transport. The present work systematically investigates segregation behaviors of aluminum (Al) and iron (Fe) impurities in YSZ grain boundaries by using molecular dynamics simulations. We have investigated the dynamics of Al and Fe impurities across two grain boundary configurations, symmetric and mixed boundaries, with respect to their relative impacts on oxygen ionic conductivity. Our findings indicate that Al impurities, because of its relatively low solubility, have a tendency to segregate extensively along the grain boundaries and, therefore, reducing significantly the ionic conductivity. On the other hand, impurities like Fe exhibit a lesser tendency to segregate and, hence, can potentially stabilize the crystal structure of YSZ without adversely impacting conductivity. Since both ions, Al and Fe, are positive ions, the barrier of ion diffusion at grain boundaries is enhanced, further affecting the overall conductivity of both species. These results improve our understanding of the impurities segregation in YSZ while providing pathways to optimize the electrochemical performance of YSZ-based devices by manipulating impurities concentrations and grain boundary engineering.



Advancing Materials Data, Design, and Discovery
April 23–25, 2025, Kyushu University, Fukuoka, Japan

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

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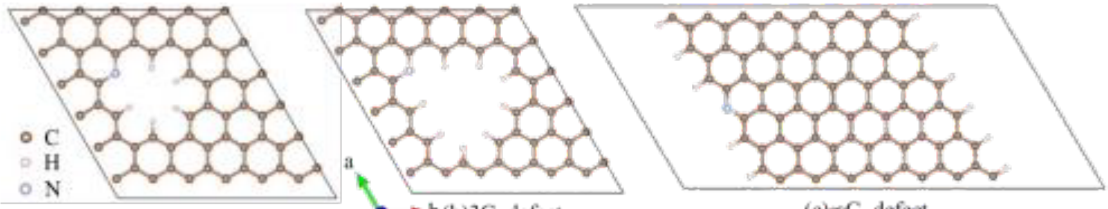
Introduction

Solid oxide fuel cells (SOFCs) have attracted significant attention as sustainable energy technology. Recently, integrated systems combining fuel cells with aquaculture have emerged as promising solutions for recouping fuel cell investment costs. In these integrated systems, aquaculture residues are fermented to generate biogas, which fuels the SOFCs [1]. However, biogas typically contains hydrogen sulfide (H_2S) impurities that poison fuel cell performance even at low concentrations. Recent research suggests that graphene-based materials, particularly those doped with nitrogen atoms, can effectively adsorb and remove H_2S from fuel streams [2]. Yet, the relationship between defect structures in nitrogen-doped graphene and their H_2S adsorption capabilities is not fully understood[3]. This study employs density functional theory (DFT) calculations to elucidate the role of graphene defect structures in enhancing H_2S adsorption and removal capabilities.

Methods

DFT calculations were performed to study graphene sheets with nitrogen-containing pyridinic defects of varying sizes. Figure 1 illustrates the defect structures, including graphene with one benzene-ring unit removed (1C6), highlighting a single benzene-ring vacancy termed "1C6," and larger defects($3C_6$ defect, and ∞C_6 defect). All computational models were constructed using periodic graphene sheets with systematically introduced nitrogen-containing defects. Adsorption energies, optimized geometries, and electronic structures were computed using the Vienna Ab-initio Simulation Package (VASP) with the Perdew–Burke–Ernzerhof (PBE) functional and projector-augmented wave (PAW) method. Also, 900 eV energy cutoff and a 4×4×1 k-point mesh were employed. Transition state search and reaction pathway analysis were conducted using the climbing-image nudged elastic band (CI-NEB) method.



(a)$1C_6$ defect (b)$3C_6$ defect (c)∞C_6 defect

Figure1. Structure of $1C_6$ defect(a), $3C_6$ defect (b), and ∞C_6 defect(c).

Results

The DFT calculations revealed that large pyridinic nitrogen defects (∞C_6 defect) enhance the adsorption property of H_2S compared to small defect ($1C_6$ defect) as seen in Figure 2, suggesting stronger binding interactions.

Moreover, reaction pathway analyses indicated that larger pyridinic nitrogen defects considerably lowered the activation barriers for the dissociation of H_2S into sulfur and hydrogen, promoting more efficient desulfurization. In contrast, smaller defects exhibited higher reaction barriers, making dissociation energetically unfavorable. These computational insights highlight the critical importance of defect size in optimizing graphene materials for efficient H_2S adsorption and dissociation for SOFCs.

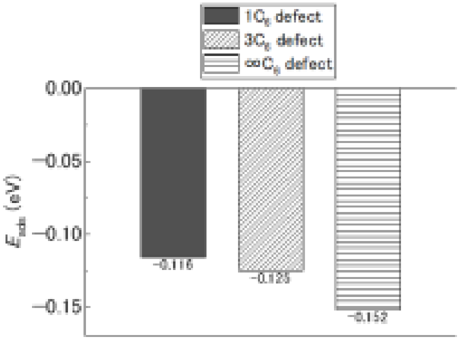


Figure 2, Adsorption energies (E_{ads}) for each crystal structures $1C_6$ defect, $3C_6$ defect, and ∞C_6 defect absorbed by H_2S.

Acknowledgments

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

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Solid-state electrolyte batteries are expected to replace liquid electrolyte lithium ion batteries in the near future thanks to their higher theoretical energy density and improved safety. However, their adoption is currently hindered by their lower effective ionic conductivity, a quantity that governs charge and discharge rates. Identifying highly ion-conductive materials using conventional theoretical calculations and experimental validation is both time-consuming and resource-intensive. While machine learning holds the promise to expedite this process, relevant ionic conductivity and structural data is scarce. Here, we present a domain-expert-curated database of ~600 synthesized solid electrolyte materials and their experimentally measured room temperature ionic conductivities gathered from literature. Each material is described by their measured composition, space group and lattice parameters. A full-crystal description in the form of a crystallographic information file (CIF) is provided for 320 structures for which atomic positions were available.

We discuss various statistics and features of the dataset and provide training and testing splits that avoid data leakage. Finally, we benchmark seven existing ML models on the task of predicting ionic conductivity and discuss their performance. The goal of this work is to facilitate the use of machine learning for solid-state electrolyte materials discovery.

Lithium-ion batteries (LIBs) used in most consumer electronics and electric vehicles have seen immense progress in terms of energy density, power density, safety and durability. However, their performance is reaching a plateau. Solid-state batteries are regarded as the next generation of batteries that may allow significant improvement over these characteristics Janek & Zeier (2016, 2023). The key difference between these two technologies is their electrolyte, the medium which allows the transport of ions during charge and discharge. A solid-state electrolyte (SSE)—as opposed to a liquid electrolyte in LIBs—permits new design choices that ultimately lead to better battery properties Betz et al. (2019), let alone the fact that solid electrolytes are not flammable unlike their liquid counterparts.

SSEs have a long research history, starting from Faraday's first discovery of fast ion transport in β-PbF_2 and Ag_2S about 200 years ago Funke (2013), until the relatively recent development of Li-based ionic conductors, such as $Li_{10}GeP_2S_{12}$ Kamaya et al. (2011).

Ionic conductivity (σ), expressed in siemens per centimeter (S/cm), measures how easily ions can move through a medium or material. Ideal SSEs, also called "superionic" or "fast-ionic" conductors, are electrolytes that exhibit ionic conductivity comparable to those observed in liquid electrolytes and molten solids (> 1 mS/cm). Only a limited number of *room temperature* ideal SSEs are known thus far within a small number of classes of materials such as LISICON (e.g., $Li_{14}ZnGe_4O_{16}$), NASICON (e.g., $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$), garnet (e.g., $Li_7Li_3Zr_2O_{12}$), perovskite (e.g., $Li_{0.5}La_{0.5}TiO_3$), and argyrodite (e.g., Li_6PS_5Cl) Janek & Zeier (2023).

Until now, the discovery of novel SSEs has largely relied on an incremental, ex perimental approach which consists, for example, of substituting atoms and elements in known compounds. This has allowed the discovery of some highly ion-conductive materials, but greatly limits the search space given that the experimental synthesis and characterization of a new, stable, inorganic solid-state electrolyte is a difficult and costly process that can take months to years Zhao et al. (2022).

Computational discovery, on the other hand, requires time-consuming atomistic simulations, such as ab initio molecular dynamics (AIMD), to accurately capture the complex relationship between ionic conductivity and the material's structure and composition Ceder et al. (2018); Qi et al. (2021); Bielefeld et al. (2020). These calculations can take from several hours to a few days for a single ionic conductivity and their parameters are often materials specific. Therefore, they are not well suited for large-scale explorations of hypothetical materials.

Machine learning (ML) has the potential to greatly accelerate the discovery of novel SSEs. Naturally, it can be used to predict ionic conductivity directly using, for example, graph neural networks (GNNs), which have been used extensively and successfully in materials science Schmidt et al. (2019); Butler et al. (2018). Machine-learned force fields or interatomic potentials (MLFF or MLIP) can also be used to obtain ionic conductivity through molecular dynamics in the "classical" way while using significantly less resources Wines & Choudhary (2024). Finally, generative frameworks can accelerate dynamics simulations Nam et al. (2024) and, provided that good ionic conductivity models are developed, there exists a wide range of frameworks that could generate new materials conditioned on that property Hernandez-Garcia et al. (2023); Zhu et al. (2024); Zeni et al. (2023); Merchant et al. (2023). However, the main obstacle to the development and validation of these models—and to some extent theoretical models—is the scarcity of relevant experimental ionic conductivity and structural datasets. Indeed, as detailed in the next section, the few datasets that exist contain partial material descriptions and ionic conductivity measurements at various temperatures. To the best of our knowledge there does not exist another open access dataset of experimental room temperature ionic conductivities with corresponding full crystal descriptions.

In this work, we assembled a curated database of 599 synthesized solid electrolyte materials and their experimentally measured room temperature ionic conductivity along with descriptors of their space group, lattice parameters, and chemical composition. The database is analyzed in terms of the distribution of ionic conductivity, space groups, elements, and repeated compositions. We also propose a training and testing split that avoids data leakage between similar entries while balancing distributions of properties across splits. We use this split to benchmark the performance of 7 machine learning models at directly predicting room temperature ionic conductivity (σ_{RT}). Our database and benchmarks aim to significantly accelerate the ML-assisted discovery of novel SSEs with fast ion diffusion.

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Intense terahertz field-induced impact ionization in narrow bandgap semiconductors

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Laser-based few-cycle terahertz (THz) radiation sources have seen significant advancements in the past 20 years, driven by major progress in intense femtosecond laser sources. More recently, scientists have developed several critical technologies to generate intense THz pulses [1-6], leading to a new field of nonlinear THz spectroscopy [7-9]. In this talk, I will review our recent results on nonlinear THz effects in narrow-band semiconductors, such as InSb and Ge. We reveal the intricate interplay between two major nonlinear THz effects, intervalley scattering and impact ionization, generated by an intense few-cycle THz pulse in an undoped (100) indium antimonide semiconductor at room temperature. Our results show an initial transmission enhancement when increasing the peak electric field to 91 kV/cm, followed by increased absorption for higher fields. Our analytical model shows that the THz strength of 91 kV/cm is the critical field. Below this field, absorption bleaching (induced by intervalley scattering of electrons in the conduction band) is dominant, whereas above it, impact ionization starts to be the dominant energy loss mechanism. The temporal and amplitude change of the total average effective carrier mass and the total carrier density allow us to monitor the THz strength fields where each scattering effect is dominant. We find that the change in the carrier populations is not the only factor that influences the current density; indeed, the average drift velocity of each valley is also a decisive factor derived from the carrier momentum change.

We have developed a theoretical model that qualitatively matches the experimental results very well. However, a quantitative discrepancy exists between the simulated and experimentally observed data, especially under conditions where impact ionization is dominant. We believe this discrepancy is due to the empirical formula we use for the impact ionization rate [10].

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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

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Electrochemical reactions provide a cost-effective and sustainable approach to converting low-value chemicals into value-added products while promoting carbon neutrality. For instance, the nitrogen reduction reaction (NRR) offers a green alternative for ammonia synthesis under ambient conditions, potentially replacing the energy-intensive Haber-Bosch process. However, large-scale implementation remains challenging due to the low activity and selectivity of electrocatalysts. To accelerate catalyst discovery, data-driven and machine-learning approaches are increasingly exploited in computational catalysis, by leveraging material databases for high throughput screening. Machine learning algorithms efficiently explore chemical space, while density functional theory (DFT) calculations provide detailed insights into the electronic structure of promising candidates. While these methods are valuable for initial screening, they do not fully capture the electrochemical environment of the catalytic process, where the electrode potential plays a crucial role. In this contribution, we present a comprehensive computational framework for electrocatalyst design for the NRR, starting with high-throughput screening of bimetallic alloy catalysts, followed by DFT characterization to assess the catalytic activity of potential candidates. To address the limitations of conventional models, we employ grand-canonical ensemble DFT (GCE-DFT) to further investigate the effect of constant electrode potential on nitrogen species adsorption and activation energies, particularly for the potential limiting step of the NRR. This approach helps paint a more realistic picture of electrochemical processes at the atomistic level, shedding light on electrocatalyst determinants for the NRR, and affording sustainable catalyst design strategies for electrochemical reactions beyond ammonia synthesis.

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

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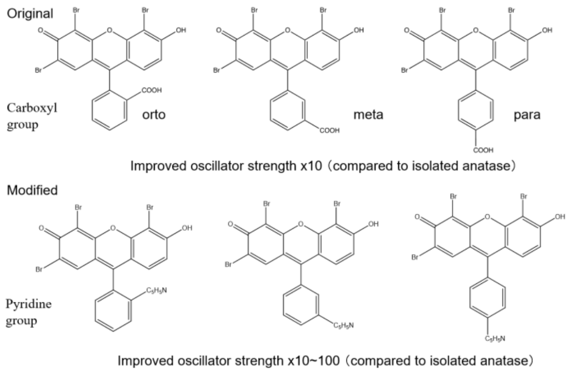
This abstract contains two parts of work describing the application of Density Functional Theory (DFT) computations to materials science research. One is in the field of chemistry, where computational studies are used to help design efficient photocatalysts. The other part is in the field of engineering, where theoretical calculations are performed to explain the mechanisms behind experimental phenomena and help understand the performance degradation of engineered materials.

1. Improved photocatalytic performance of eosin Y-sensitized anatase by anchoring group modification.

A great number of attempts on H_2 production from water using photocatalyst have been made to construct solar energy conversion systems to chemical energy. Eosin Y-sensitized anatase has been identified as an efficient photocatalyst because of its activity in visible light [1]. Though eosin Y having carboxyl groups could be fixed by ester-like linkage on anatase in the organic solvent, the linkage was not stable in water because of hydrolysis [2]. In order to overcome the unstableness of the eosin Y-sensitized anatase in water, we attempted a strong chemical fixation of dye on anatase particles. We proposed the use of a pyridine ring as an anchoring group in place of a conventional carboxyl group.

Comparative study on the hybrid interface of anatase and eosin Y with the different anchoring groups were performed by density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations. The geometries, binding interaction between dye and anatase, electronic structures and transfer as well as the effect of isomers (orto-, meta, para-) on the dye-anatase systems were investigated and discussed. Theoretical results indicated that EY with carboxyl and pyridine anchors had visible adsorption and electron transfer from the dye to the particle. Compared to carboxyl-para, which had the best optical performance among carboxyl groups, the adsorption strength of pyridine-orto was close to that of carboxyl-para, while the oscillator strength increased significantly, which was more than 10 times higher than that of carboxyl-para. Non-equilibrium Green’s function (NEGF) method was successfully employed to elucidate the distinctive electron transport in the pyridine-linked molecular junction compared to the carboxyl-linked junction. This study provides a potential design for EY-sensitized anatase in photoelectrochemical water splitting application, where the binding strength and photocatalytic activity were improved simultaneously.



2. Enhanced hydrogen-induced degradation of pipeline steels by the CO_2 mixing in hydrogen environments

Many countries are trying to or have already blended hydrogen into the existing natural gas pipeline network to transport and use hydrogen efficiently. However, hydrogen atoms are easy to enter into metals, resulting in a large internal hydrogen concentration in the material [3]. Under the right conditions, hydrogen can degrade the mechanical properties of pipeline steels, which is known as hydrogen embrittlement (HE) [4]. HE can be a very complicated process and is a potential threat to the safety of HENG pipelines. The HE behavior of pipeline steels in the actual hydrogen-enriched natural gas (HENG) is important in evaluating the feasibility of mixing hydrogen into natural gas grids.

Our studies found that CO_2 contained in HENG could significantly enhance the HE of pipeline steels. Further, the enhanced sensitivity of pipeline steel to HE induced by the CO_2 effect is pressure dependent. The CO_2 effect at low pressure was more pronounced than that at high pressure. To elucidate what kind of role CO_2 play in the hydrogen uptake in metals, DFT calculations were performed to characterize hydrogen-metal interactions in the CO_2-free and CO_2-containing systems. Results show that CO_2 can strengthen the adsorption of H_2 and fasten the dissolution (migration from surface to subsurface) of the H atom when CO_2 is adsorbed on the iron surface. Due to the fast adsorption of H_2 itself, the promoted H dissolution rate by CO_2 is the major reason for the enhanced hydrogen uptake and HE of the steel. First-principles molecular dynamics calculations indicate CO_2 adsorption rate on the iron surface decreased with increasing hydrogen pressure. Due to the inherent rapid entry of hydrogen into material at high pressure, the slow adsorption rate of CO_2 in high-pressure CO_2-enriched hydrogen mixtures could not enhance hydrogen uptake significantly.

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Density functional theory study of electrical properties of misfit dislocations in $SrTiO_3$

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(joint work with Marivi Fernández-Serra and Andreas Ruediger)

Nearly 200 years after the discovery of the first perovskite and subsequent thorough investigations, these materials are still relevant today. Applications ranging from solar cells [1] to neuromorphic devices [2] and the resulting demand for novel material compositions resulting from this led to a steep increase in publications in this field [3]. One prominent candidate that has been under investigation for decades is $SrTiO_3$. This material is often used as a model system for complex solid-state phenomena. On the one hand, there are well-established applications, such as the use as dielectric in capacitors [4] or the use of substrates [5]. On the other hand, phenomena like superconductivity [6] or quantum paraelectricity [7] are still missing an explanation. Possible explanations often connect structural and electrical properties. Hereby, complex phonon-electron interactions are introduced that still lack validation.

In this work, we present a defect-based approach. Hereby, the coupling of properties and therefore certain effects are caused by defects and are not a property of the entire bulk structure. Defects of particular interest are dislocations. The dislocation density in $SrTiO_3$ is around $10^6\,\mathrm{cm}^{-2}$ but can be higher under mechanical stress [8]. These linear defects cause an abrupt change in the arrangement of atoms and can distort the lattice in the nanometer range. Along dislocations, experiments show a high concentration of oxygen vacancies which results in an enhanced conductivity in the normally non-conductive $SrTiO_3$ [9]. Oxygen vacancies are also a fundamental component of existing explanations and underline the importance of dislocations [10]. Furthermore, dislocations open up the possibility of investigating further effects like flexoelectricity or Raman scattering.

Dislocations in $SrTiO_3$ were already investigated experimentally and theoretically [9, 11]. However, theoretical studies either focus on structural properties using molecular dynamics simulations [12] or electrical properties using density functional theory (DFT) [13]. One problem with existing DFT studies is the use of very simplified structures in order to keep the computational time low [13]. These structures are basically vacancy structures, as visualized in Figure 1a, that miss the two key points of dislocations: change in atomic arrangement and the existence of a strain gradient with a non-zero Burgers vector. Especially the formation energy of vacancies is heavily influenced by strain [14]. In order to overcome the problem we use the DFT code SIESTA [15] which supports linear scaling for large systems allowing us to calculate realistic structures, shown in Figure 1b, and obtain insights into the structural as well as electrical properties.

The $SrTiO_3$ dislocation shows a significant strain of approximately 10 % around the dislocation core. This strain value would be impossible to introduce globally in the bulk phase without destroying the material. This results in a local polarization of up to 75 µC cm^{-2}. This polarization is even stronger than that in the polar tetragonal phase of $BaTiO_3$ with a value of 26 µC cm^{-2} [16].

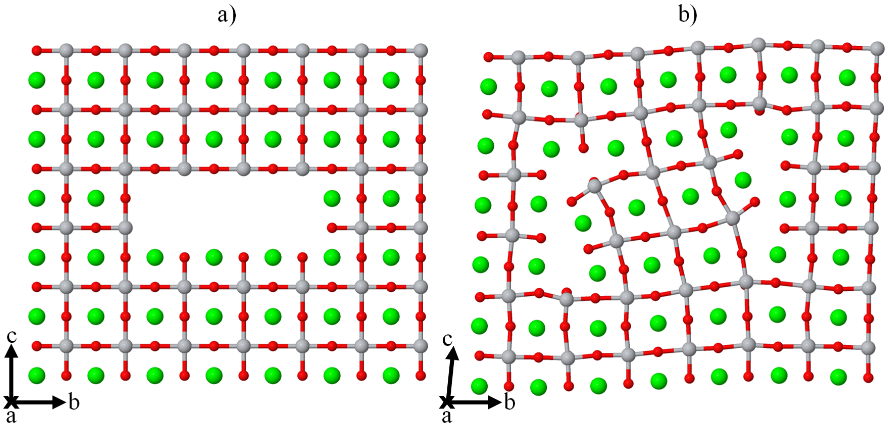

FIGURE 1. a) Simplified representation of a trivial $SrTiO_3$ dislocation used in existing DFT studies [13]. b) Realistic $SrTiO_3$ dislocation geometry used in this work. A double dislocation is used in order to enable periodic boundary conditions.

The resulting electrical properties also undergo major changes. The band gap decreased from 2.26 eV for the bulk phase to 1.94 eV caused by additional states oxygen 2p states in the valence band.
The calculations also show a drastic reduction in the formation energy of oxygen vacancy. In bulk $SrTiO_3$ the simulated formation energy is 8.53 eV. At the dislocation core, the formation energy is as low as 6.80 eV. Assuming that the formation of vacancies is a thermally activated process following the Arrhenius equation, the rate for vacancy formation at the dislocation is 31 magnitudes higher at 300 K compared to the bulk phase.

The results of this defect-based approach can indeed confirm experimental findings and give quantitative insights into fundamental processes. The aim of further simulations will be the determination of the oxygen vacancy location, whether they appear in a chain or in a zig-zag pattern along the dislocation as well as the conduction mechanism, especially the formation of polarons.

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Accelerating Molecular Discovery with Game AI methods and Supercomputers

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Molecular Discovery with Monte-Carlo Tree Search and Machine Learning

We present ChemTSv2 [2], our novel framework that combines Monte-Carlo Tree Search (MCTS) with advanced machine learning models to accelerate the discovery of novel molecules. Our approach harnesses the strengths of both simulation-based and data-driven evaluation methods, thereby creating a powerful tool for navigating vast chemical spaces efficiently. Initially devised for Go, a two-player game popular in East Asian countries, MCTS has evolved into one of the standard algorithms for solving problems from various domains, including molecular design, highlighting its cross-domain applicability and potential for future multidisciplinary challenges.

Overview of the Methodology

At the core of ChemTSv2 is an MCTS algorithm that incorporates machine learning models at multiple stages. In its original context in Go, MCTS evaluates numerous possible moves to find the optimal strategy; in our framework, it systematically explores chemical structures. We begin with generative models that quickly propose candidate molecules. Then, during the simulation (or rollout) phases of MCTS, each candidate is evaluated using two complementary methods:

- **Fast, Data-Driven Evaluations:** Machine learning predictors rapidly (within milliseconds) estimate key molecular properties, such as electronic and optical characteristics. This swift feedback is critical for guiding the search through the extensive chemical space.
- **Detailed Simulation-Based Evaluations:** For higher precision, we employ quantum chemical calculations using tools like Gaussian v16. Although these computations can take several minutes per molecule, they provide accurate assessments of properties—including excitation energies, stability, and reactivity—that are essential for material design and validation.

This approach allows ChemTSv2 to overcome a common limitation of purely data-driven methods. Traditional machine learning models often generate molecules resembling their training data (the out-of-distribution problem). In contrast, our MCTS-based approach can explore diverse and unexpected chemical structures, just as recent advanced Go programs have generated novel strategies that defy human intuition.

High-Performance Computing and Parallelization

The enormity of chemical space presents a significant computational challenge. To manage this, we have developed a massively parallelized version of our MCTS algorithm [1]. Running ChemTSv2 on supercomputers enables us to execute hundreds or thousands of simulations concurrently, dramatically reducing the overall search time and allowing us to tackle more complex materials design problems.

Results and Current Achievements

Our research has yielded promising results, including identifying several novel fluorescent molecules [3]. These initial successes demonstrate that integrating MCTS with machine learning is effective for novel findings that conventional screening methods might have overlooked. Our code is publicly available and is used by many research teams. By sharing our tools and methodologies, we aim to foster further research in material informatics and algorithmic search, inviting the community to explore new applications and improvements.

Future Directions and Broader Implications

Our goal is to refine and extend this tool to address broader challenges. One immediate direction is to improve our algorithms to better capture the multi-objective aspect of molecular discovery by considering multiple factors, such as stability, toxicity, and synthetic feasibility.

Moreover, the design of the parallel MCTS algorithm is inherently modular, suggesting that it could be generalized to other domains that require efficient exploration of large, complex search spaces. Our code currently contains chemistry-specific parts, but we can use the code base to parallelize many other MCTS applications with little modification.

Conclusion

In summary, our work demonstrates how algorithms from game AI—specifically, Monte-Carlo Tree Search—can be repurposed and augmented with machine learning techniques to revolutionize the field of molecular discovery. By leveraging both fast machine learning predictors and high-accuracy simulation tools, and by harnessing the power of supercomputing for parallel execution, we have developed a framework for identifying novel molecules. The implications of this work extend beyond chemistry, offering the potential for developing efficient, scalable search algorithms applicable to a wide range of scientific and engineering problems.

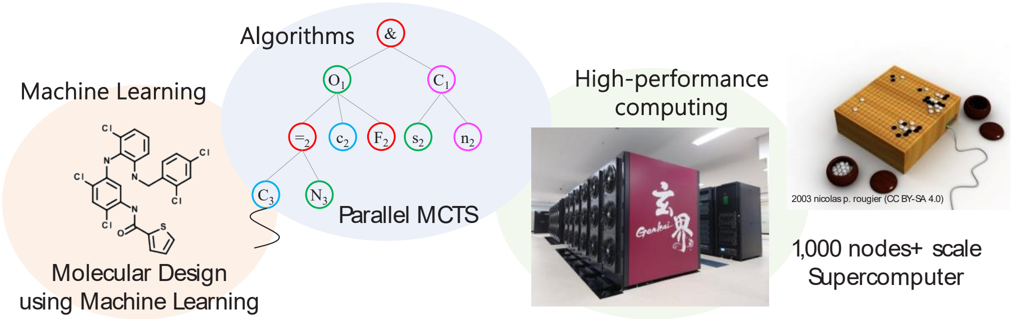

Figure 1. Our approach combines Algorithms, Machine Learning, and HPC.

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

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High-entropy alloys (HEAs) are alloys having configurational entropies exceeding 1.5*R* (*R*: gas constant) [1]. HEAs have emerged as new solid-state hydrogen storage materials but reversible storage at room temperature is still a challenge [2]. The ability of HEAs to store hydrogen at room temperature depends on Gibbs energy which is dependent on formation enthalpy (ΔH). The prediction of hydride formation enthalpy is thus the key issue in the design of new HEAs for room-temperature hydrogen storage. In this study, the formation enthalpy (ΔH) for model AB_2-type (A: hydride forming, B: non-hydride forming) HEAs ($Ti_xZr_{2-x}CrMnFeNi$, for $x = 0.5$, 1.0 and 1.5) was predicted through machine learning (ML) and the results were validated through experiments and density functional theory (DFT).

For modeling machine learning a dataset of 420 data was used. The data were curated using the leverage method. Gaussian process regression (GPR) was used to train the data using 4 different kernels. The validation of the model was done using *K*-fold cross validation and self-validation. For DFT calculations, a 48-atom supercell of Ti-Zr-Cr Mn-Fe-Ni HEAs with the C14 Laves phase was modeled. Ti and Zr were placed at A sites whereas other elements were placed at B sites. For the modeling of high-entropy hydride, it was assumed that AB_2-type HEA forms AB_2H_3-type high-entropy hydride and hydrogen occupies A_2B_2 sites ensuring minimum repulsion between hydrogen atoms. For the experimental approach, the synthesis of HEAs was done using arc melting equipment. Characterization of HEAs were done using X-ray diffraction (XRD) and scanning electron microscope (SEM). Pressure-composition-temperature (PCT) isotherms, as shown in Fig. 1 (a), were obtained at different temperatures using Sievert type equipment, using van't Hoff plot as shown in Fig. 1(b), the formation enthalpy was calculated for the HEAs.

The predicted ΔH through ML algorithm Gaussian process regression using exponential kernel are -32.1 kJ/mol, -27.7 kJ/mol and -22.0 kJ/mol for $x = 0.5$, 1.0 and 1.5 respectively. The values are consistent with experiments and DFT as shown in Fig. 1(c). It is concluded that for Ti-Zr-based HEAs, the formation enthalpy becomes less negative with the increase in Ti content [3]. Experimental results indicate that the room temperature hydrogen storage performance of HEAs is primarily governed by enthalpy rather than entropy, highlighting enthalpy prediction as the key factor in HEA design.

This study presents ML as a fast and reliable method for designing HEAs with hydride formation enthalpies ranging from −25 to −39 kJ/mol, optimized for room-temperature hydrogen storage.

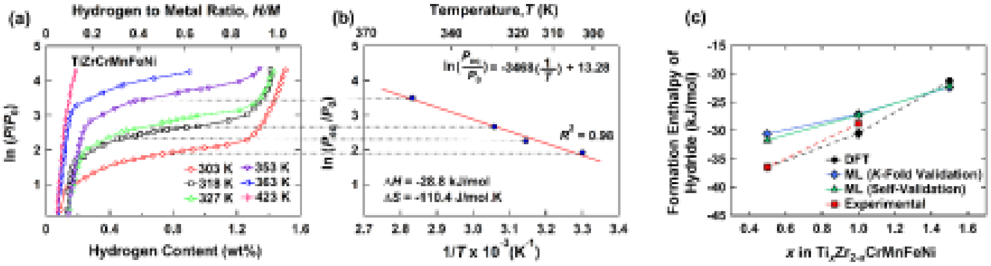

Figure 1 (a) Pressure-composition-temperature isotherms and (b) corresponding van't Hoff plot for TiZrCrMnFeNi HEA. (c) Comparison of ΔH using ML, experiments, and DFT.

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

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The development of proton-conducting electrolyte materials is crucial for the realization of the next-generation fuel cells that operate at intermediate temperatures (300-450°C). Proton-conducting ceramics have traditionally been developed based on trial-and-error experiments relying on exploration in the analogous system to the well-known materials or researchers' intuition. However, this process is time-consuming because of the broad space for searching in chemistry. Here, I present the success in the efficient development of novel proton-conducting ceramics, $SrSn_{0.8}Sc_{0.2}O_{3-\delta}$, utilizing small experimental data and machine learning [1].

We predicted the proton concentration in hypothetical perovskite oxides by the Gradient-boosting regressor using the reliable literature data and the experimental data we obtained. The database includes 761 data for 65 compounds with various experimental conditions (temperature, water partial pressure, etc.). By selecting the reliable candidate utilizing a descriptor-target map, we could choose the $SrSn_{0.8}Sc_{0.2}O_{3-\delta}$ by the first experiment trial. The blue plots in Figure 1 show the temperature dependence of predicted proton concentration, whereas the red ones depict those of experimental results in $SrSn_{0.8}Sc_{0.2}O_{3-\delta}$. The predicted and measured data agreed well, especially at high temperatures. The developed materials show relatively high proton conductivity at ~1 mS·cm^{-1} at 338°C, demonstrating the efficient discovery of novel electrolyte material utilizing machine learning prediction.

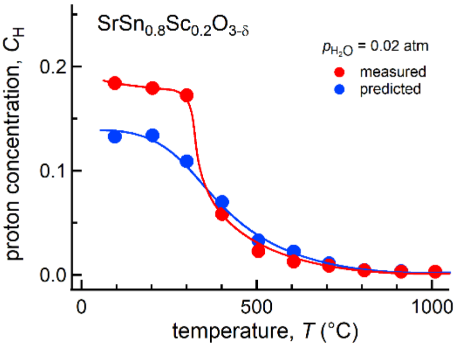

Fig. 1 Temperature dependence of predicted (blue) and measured (red) proton concentration in $SrSn_{0.8}Sc_{0.2}O_{3-\delta}$.[1]

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

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In the course of the years the phenomenon known as *remodeling* has catalyzed the attention of an increasing number of scientists working in theoretical, computational and applied biomechanics. According to the definition given by Taber [1], *remodeling* is understood as the process by which a living tissue is capable of transforming its internal structure. The structural transformations that may occur can be of various kind and, although they can all be viewed as the manifestation of the activation of some peculiar structural degrees of freedom, the origin of such activation covers events of genetic nature, interactions taking place at the cellular and intercellular level, and interactions involving the tissue as a whole with its surrounding world.

Each type of interaction that concurs to the remodeling of a tissue is marked by certain mechanical, physical and chemical aspects, which, in turn, are characterized by their own time- and length-scales. These become even more important when remodeling takes place in biological media that, because of their particular internal structure and geometry, can be envisaged as composite materials featuring two or more phases, well separated by sufficiently sharp interfaces. In this case, the structural transformations can be directly associated with the phases constituting the composite under study, and the interphase interactions, occurring at the interfaces, assume a very precise role in the determination of the macroscopic behavior of the tissue as a whole.

Among the various forms that remodeling can take, in this contribution we focus on the case in which it is a mere mechanical process. In particular, we consider a bio logical composite material constituted by two solid phases that, under the action of mechanical stimuli, undergo deformations and inelastic distortions. Although both are studied at the scale of each phase (thus, at the scale identified with the microscopic one), the inelastic distortions are assumed to represent a structural reorganization that pertains to lower scales, not explicitly resolved.

For our purposes, we consider an “idealized” hierarchical medium, which could be regarded as a very essential approximation of bone tissue, and we base our study on the hypothesis that the internal structure of the medium is obtained by indefinitely repeating a “representative cell”. Hence, the idealized composite has periodic internal structure and its “representative cell” has the property of condensing in itself all the most relevant pieces of information about its geometry and mechanical behavior.
Within this setting, we attribute the evolution of the inelastic distortions representing remodeling to the generation of irreversible strains in the medium, which could be due,

for example, to damage. In the literature, this type of process is often studied in analogy with the theory of finite strain plasticity (see, e.g., [2]). In our contribution, however, we take a step forward, and we make the fundamental hypothesis that the inelastic distortions vary spatially over a length scale covering more representative cells of the composite. A case of biomechanical interest in which such a condition is verified is given in [3].

To account explicitly for the spatial variability of the inelastic distortions, we resort to the theory of strain gradient plasticity put forward by Gurtin&Anand [4], and we adapt it to our context. Above all, given the periodic structure of the composite material at hand, we perform the two-scale Asymptotic Homogenization of the model equations. This leads to the determination of an *effective*, homogenized version of the composite, the mechanical response of which is characterized by effective elastic and viscoplastic parameters. In doing this, we also provide a homogenized version of the *flow rule* that, in the model put forward in [4], governs the evolution of the inelastic distortions.

To reduce the complexity of the calculations, we consider the particular case of a laminated, multi-layered composite material under uniaxial loading and symmetric boundary conditions.

The contents of this contribution and of the related presentation constitute some of the main results of a recent work of ours [5].

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Dislocation and disclination in crystalline materials: a differential geometry approach

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Dislocations and disclinations are one-dimensional lattice defects in crystalline materials, often referred to as Volterra defects. They represent the breaking of translational T(3) and rotational SO(3) symmetries in periodic structures. Recently, we have modeled Volterra defects using differential geometry on a Riemann-Cartan manifold [1-3].

First Study: Screw Dislocation Modeling [1]
Our initial work focused on the theoretical modeling and numerical analysis of screw dislocations. By expressing Cartan's first structure equation in variational form and solving it numerically using isogeometric analysis, we successfully modeled arbitrary dislocation configurations. Additionally, we solved the elastic embedding from the intermediate to the current configuration by minimizing the strain energy functional via IGA. This approach removed the stress singularity by relaxing the dislocation core structure from a Dirac delta function to a continuous function. Our findings revealed localized nonlinear stress fields around the dislocation core, with a decay rate scaling as $1/r^2$, significantly higher than the classical 1/r scaling. Furthermore, the geometric frustration within the dislocation core was expressed in terms of Ricci curvature rather than torsion. We demonstrated that the six components of Ricci curvature exhibit rotational symmetries consistent with stress symmetries, confirming the long-standing hypothesis of stress-curvature duality.

Second Study: Plastic Deformation and Electromagnetic Analogy [2]
In the second study, we modeled specific dislocation densities using Cartan's first structure equation. Through Helmholtz decomposition, we extracted the plastic part of the displacement gradient, a key element of plastic deformation fields. This decomposition aligned Cartan's equations and the divergence-free condition with Ampère's and Gauss' laws in electromagnetics. Consequently, the Biot-Savart law for static magnetic fields was adapted to describe plastic mechanics. This mathematical analogy provided analytical solutions for both screw and edge dislocations, independent of their type. Additionally, the governing equations for plastic deformation were shown to correspond to the Cauchy-Riemann equations in complex function theory. The plastic potential, expressed as a complex function, displayed multivalued behavior discretized by integer multiples of the Burgers vector. These findings underscored the differential topological nature of dislocations, beyond their geometric classification. Elastic stress fields generated by plastic deformations, derived analytically, were consistent with Volterra dislocation theory, linking the stress fields directly to geometric frustration described by Einstein curvature.

Third Study: Unified Modeling of Volterra Defects [3]

In our third study, we developed a mathematical framework for Volterra defects using Riemann-Cartan manifolds. Translational and rotational deformations were introduced as Volterra deformations along coordinate axes, with Cartan's moving frame representing the plastic deformation field. By applying the Weitzenböck connection to Cartan's equations, we confirmed that dislocation densities align with classical lattice defect definitions. For disclinations, the presence of excess torsion or curvature components suggested the need for modifications in the Volterra process. The non-uniqueness of connections in the Riemann-Cartan manifold allowed flexibility in switching between Weitzenböck and Levi-Civita connections, establishing a geometric equivalence between dislocations and disclinations. Analytical solutions using the Biot-Savart law demonstrated the existence of wedge disclinations at the termini of edge dislocation arrays, with edge dislocations acting as the momentum of wedge disclination dipoles. We also showed that isolated wedge disclination monopoles can form with semi-infinite edge dislocation arrays. The plastic deformation fields of wedge disclinations were shown to be conformal, representable by orthogonal coordinate systems. Riemannian holonomy quantitatively measured the Frank vector of disclinations, and complex potentials further elucidated their topological properties, including jump discontinuities. Analytical stress field solutions, consistent with prior studies, highlighted the robustness of this geometric framework.

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

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Since their initial discovery, luminescent rare earth-doped nanoparticles have garnered significant attention. Over the past decade, the field has experienced rapid advancement, moving from a fundamental understanding of the photophysical mechanisms underlying their nanoscale luminescence, especially upconversion, to their application across a wide range of fields, with notable emphasis on biology and medicine. This growing interest is largely due to their ability to be excited by near-infrared (NIR) light and their diverse emission spectra, which range from the UV to the NIR. Consequently, a single NIR excitation can produce either higher-energy luminescence (upconversion) or single-photon NIR emission (down-shifted luminescence). The upconversion process occurs through the sequential absorption of multiple NIR photons via the long-lived 4f electronic states of trivalent rare earth ions, making it several orders of magnitude more efficient than conventional multiphoton absorption. This is particularly promising for theranostic (therapy + diagnostic) applications, where the upconverted light can activate therapeutic modalities (e.g. drug release or photodynamic therapy), while NIR luminescence serves for diagnostic purposes (e.g. bioimaging and nanothermometry). In this work, we present our progress on the synthesis and development of multi-functional, rare earth-doped nanoplatforms, demonstrating how their various emissions can be harnessed for biological and medical applications.

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Accelerating Material Discovery through an Automated and Data-Driven Workflow

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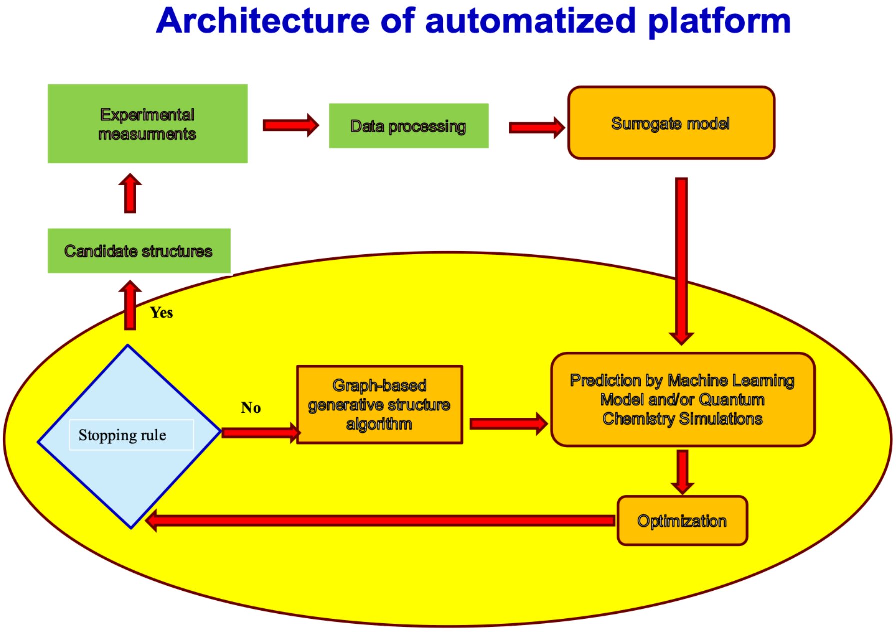
Abstract

The discovery of novel materials with desirable properties is a critical challenge in materials science. Material discovery is often hindered by the complexity and cost of experimental trials. To address this, we have developed an automated workflow that integrates mathematical modeling, computational algorithms, and data-driven techniques to optimize the material discovery pipeline. This platform is designed to systematically identify promising candidates with enhanced efficiency. Its versatility is demonstrated through applications in diverse material systems, including photo-resisting monomers, diarylethene molecules, and austenitic alloys, each exhibiting distinct properties. The results highlight the potential of this approach in streamlining material discovery. Future developments will focus on extending the platform to more complex systems, further enhancing its capability to tackle intricate material design challenges.

Workflow



The discovery of new materials is a multifaceted challenge that requires integrating computational and experimental techniques. Our platform streamlines this process by incorporating automated data analysis, machine learning models, and high-throughput simulations. The workflow begins with a small set of experimental data, which serves as the foundation for further computational exploration. This data undergoes preprocessing to extract key information relevant to the target properties. The above graphical diagram illustrates the workflow, demonstrating how different components interact to optimize the material discovery process.

1. Surrogate Modeling for Efficient Material Screening

One of the core components of our approach is the construction of a surrogate model. A surrogate model acts as an approximation method, particularly useful when the desired outcome is challenging to measure or compute directly. By leveraging this model, we can predict the properties of new candidate materials with high accuracy, reducing the need for costly and time-consuming experiments. This predictive capability is especially beneficial for identifying materials with optimal properties in a high-dimensional design space.

2. Graph-Based Evolutionary Algorithm for Molecular Design

Another essential submodule of our platform is the graph-based evolutionary algorithm. This algorithm systematically mutates molecular structures to generate a large number of candidates in each iteration step. Molecules are represented as graphs, where atoms are nodes and bonds are edges. The algorithm ensures chemical validity while maintaining diversity in the generated structures. This systematic exploration of the molecular design space is critical for discovering promising candidates that may not be apparent through manual or random approaches.

3. Automated Quantum Chemistry Workflow

To further enhance the efficiency of our platform, we developed an automated Python program that controls Turbomole quantum chemistry calculations via the ASE (Atomic Simulation Environment) Python wrapper. This program demonstrates the power of automation in handling large-scale quantum chemistry calculations.

4. Performance of Graph Convolutional Neural Network Models

We constructed Graph Convolutional Neural Network (GCN) model for predicting the properties of DFT calculation which hep reduce the computational cost. The results indicate that the model achieves sufficient accuracy for real applications. The validation from industry underscores the practical value of our approach in supporting real-world material discovery efforts. The integration of machine learning into our pipeline not only enhances prediction accuracy but also enables the identification of complex structure-property relationships that are otherwise difficult to discern through traditional methods.

Conclusion and Future Work

Our automated and data-driven workflow presents a promising approach for accelerating material discovery. By integrating surrogate modeling, evolutionary optimization, and high-throughput quantum chemistry calculations, we can efficiently explore vast chemical spaces and identify novel materials with desirable properties. Future work will focus on extending the platform to more complex material systems and further refining the predictive models to enhance accuracy and generalizability. The success of this approach highlights the transformative potential of automation and machine learning in materials science.

Reinforcement learning for self-assembly problems

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(joint work with Uyen Tu Lieu)

Self-assembly is a phenomenon in which particles move collectively and form a structure with order. Controlling self-assembly structures is a key challenge in materials science to make materials with useful physical properties. This problem also has various interesting aspects in fundamental sciences, such as the characterisation of ordered structures and the mechanism of structural formation from a disordered state. These issues are hot research topics, particularly in soft condensed matter physics, statistical mechanics, and nonlinear dynamics[1, 3]. In equilibrium systems, target structures can be tailored by a functional form of their free energy. Although the quantitative design of the equilibrium structures is still challenging, several systematic approaches have been proposed. On the other hand, designing out-of-equilibrium structures remains elusive, despite the fact that most of the materials' production processes are in non-equilibrium states. In this case, the aim is to find an optimal parameter change as a function of time during the self-assembly process.

Recently, machine learning techniques have been applied to self-assembly problems. For example, interaction between colloidal particles can be optimised so as to reproduce desired structures[2, 4]. Using those approaches, we can figure out what kind of interaction (symmetry, distance dependence) is necessary to form complex structures, such as quasicrystals. However, those designs are limited to the static parameters of the systems.

In this study, we propose the method of optimal feedback control to make a desired structure[5]. Specifically, we consider the colloidal self-assembly into quasicrystals by controlling the temperature. Using the framework of reinforcement learning, we estimate the policy, namely, how the temperature should be changed in the next time step after measuring the current structure. We demonstrate that our estimate policy generates quasicrystals more efficiently than using the conventional annealing or quenching method. We also show that we can dynamically stabilise not only stable structures but also metastable and even unstable structures.

The basic idea of reinforcement learning is to estimate the best policy to reproduce the target structure. To do this, we consider a tuple of state s_t at time t, action a, Markov transition dynamics of structure $P(s_{t+1}|s_t, a)$, instantaneous reward r_t, and policy $\pi(a|s_t)$(Fig.1). In our study, the policy is whether temperature goes up, stays, or goes down as a function of the state (Fig.1(B)). Once we estimate the best policy, we may dynamically change the temperature following the policy, and then obtain the structure close to the target (Fig.1(A)). We use Q-learning to train the policy. In this method, we use the Q-function (Q-table) $Q(s_t, a)$, which is the expected value of future reward under the action, a. The instantaneous reward is evaluated by comparing the structure obtained from experiences and the target. Then, we can iteratively update the Q-function by numerically solving the Bellman's equation, namely, minimising the difference between $Q(s_t, a)$ and its expected value at the next step $r_{t+1} + \gamma \max_a Q(s_{t+1}, a)$.

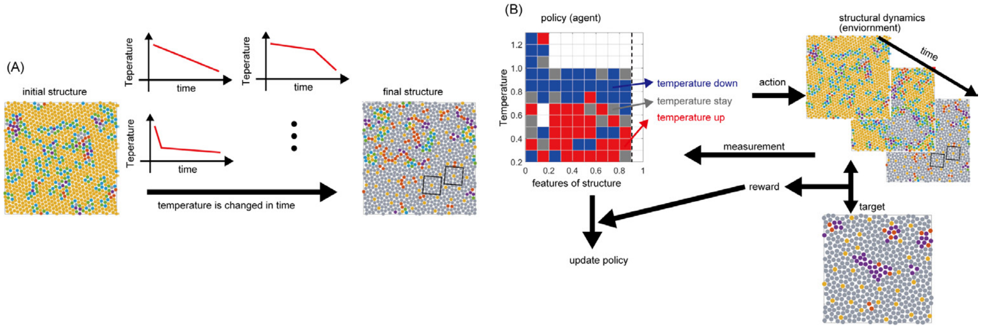

FIGURE 1. Schematics of reinforcement learning for the self-assembly of colloidal particles.

The estimated policy for the self-assembly of particles is shown in Fig.1(B). The particles are in two-dimensional space and are interacting with each other through five-fold-symmetric anisotropic potential. The target structure is a two-dimensional dodecagonal quasicrystal. The previous studies revealed that this structure cannot be reproduced by rapid cooling (quenching), but can be reproduced by slow temperature change (annealing)[3]. Using our estimated policy, we are capable of reproducing the quasicrystalline structure in a faster time scale than annealing (Fig.2). The policy indicates that there is a characteristic temperature at which we should switch the policy of temperature increasing and decreasing. This means that we should first change the temperature to the transition temperature at which structural fluctuation is enhanced. Once we obtain the quasicrystalline structure, we should decrease the temperature to stabilise it.

We emphasise that we did not feed the information of the transition temperature into reinforcement learning. Still, our method automatically found it and optimised the policy so that we could reproduce the target more effectively. So far, reinforcement learning is rarely used in the self-assembly problems, but we believe that our method is useful for future design of the process of self-assembly, and there is also a deep physics behind the success of this method.

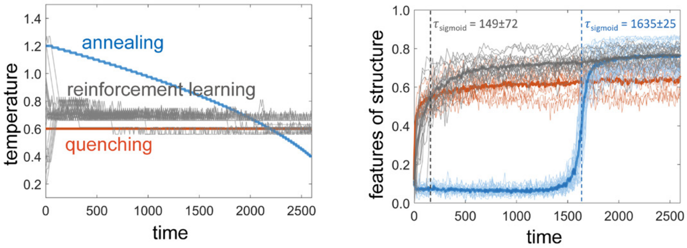

FIGURE 2. (A) Temperature change in time using th estimated policy (grey), annealing (blue), and quenching (orange). The feature of the structure measuring how it is close to a dodecagonal quasicrystal under different temperature change.

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Multicellular simulations with shape and volume constraints using optimal transport

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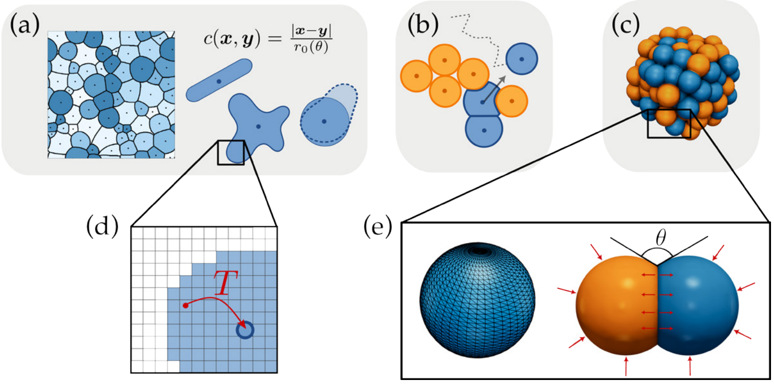

FIGURE 1. **Graphical abstract.** (a) Laguerre tesselations generalize Voronoi diagrams with volume, shape and deformation constraints using a cost function c. (b) Any active point-particle model can be enriched with volume exclusion and arbitrary deformability properties. (c) The framework is implemented in 2D and 3D. (d) Laguerre tessellations are computed as the solution of a semi-discrete optimal transport problem on a discrete grid. (e) In 3D, a meshing of each cell boundary is computed in order to implement surface tension effects.

1. INTRODUCTION

Many living and physical systems such as cell aggregates, tissues or polycrystalline materials behave as unconventional systems of particles that are strongly constrained by volume exclusion and shape interactions. Understanding how these constraints lead to macroscopic self-organized structures is a fundamental question in particular in developmental biology. To this end, various types of computational models have been developed, including phase-fields [18], level-set methods [21], cellular automata [14], Voronoi tessellations [1], vertex models [15], finite elements methods [5, 19] etc.

In [11], we have introduced a new framework to model particle systems with arbitrary dynamical shapes and deformability properties. As a starting point, our method revolves around an independent volume constraint for each particle. Indeed, although volume is the first experimentally measurable quantity, most of the approaches mentioned above provide little control on it, as it is usually treated as a soft constraint. As a first description, our method can be seen as a generalized Voronoi tessellation method with strict volume constraints. To achieve this goal, we rely on the notion of Laguerre tessellation which has recently appeared in various different contexts, in particular the simulation of incompressible fluid flows [4, 13, 16], of crowd motion [17], the modeling of polycrystalline materials [2, 3, 7] and in computer graphics [10, 6]. Although apparently fundamentally different, these situations are actually related to the theory of optimal transport which offers both a well-studied mathematical framework and state-of-the-art GPU implementation techniques.

Although our model is formally a tessellation model, it shares important properties with point-particle systems, level-set methods and vertex models, which thus also suggests a novel optimal transport point of view for these methods. As a consequence, our model is remarkably versatile: within the same framework, we can represent individual particles with arbitrary shapes (as in level-set methods), their collective motion (as in point-particle systems) and much denser tissue-like aggregates whose dynamics is ruled by surface tension and other contact-based interactions.

An extended gallery of examples alongside our open source implementation can be found on the documentation website

`https://iceshot.readthedocs.io/`

2. Model

We consider a set of $i = 1, \dots, N$ particles, each of them defined by the couple $(\boldsymbol{x}_i, v_i)$ of its position, in a given domain Ω of size 1, and its volume. Each particle i is modeled by a *Laguerre cell* $\mathscr{L}_i$, defined as the following set of points:

$$\mathscr{L}_i = \{\boldsymbol{x} \in \Omega,\ c(\boldsymbol{x}, \boldsymbol{x}_i) - w_i \leq c(\boldsymbol{x}, \boldsymbol{x}_j) - w_j \text{ for all } j\}. \tag{1}$$

- The function $c : \Omega \times \Omega \to [0, +\infty)$ is an arbitrary function, called *cost function*, which encodes both the shape and the deformability properties of each individual particle. A typical example to keep in mind is the L^2 cost defined as the square of the distance function: $c(\boldsymbol{x}, \boldsymbol{y}) = |\boldsymbol{x} - \boldsymbol{y}|^2$.
- The *Kantorovich potentials* $w_1, \dots, w_N$ are uniquely defined in order to satisfy the volume constraint $\mathrm{vol}(\mathscr{L}_i) = v_i$.

For a large class of cost functions and any positions $\boldsymbol{x}_i$, the Laguerre tessellation (1) can be shown to be the unique solution of the following constrained minimization problem on the set of partitions of Ω:

$$\mathcal{T}_c = \min_{(\mathscr{L}_i)_{i=1,\dots,N}} \left\{ \sum_{i=1}^{N} \int_{\mathscr{L}_i} c(\boldsymbol{x}, \boldsymbol{x}_i) \mathrm{d}\boldsymbol{x},\ \text{ with constraints } \mathrm{vol}(\mathscr{L}_i) = v_i \right\}.$$

In optimal transport theory, such partition is understood as an assignment problem, where each point $\boldsymbol{x} \in \Omega$ is assigned to one of the $\boldsymbol{x}_i$ at a cost $c(\boldsymbol{x}, \boldsymbol{x}_i)$. This interpretation provides a fast numerical method to compute the Kantorovich potentials w_i [12, 8]. When c is the L^2 cost and $w_i = 0$, we recover the standard definition of a Voronoi diagram. Generalizing the distance function into an arbitrary function c is a key modeling idea which allows arbitrary shapes, defined as level-sets of the cost function, and boundaries between neighboring particles, defined by algebraic equations.

In a dynamical framework, we consider the following first-order gradient descent equation for the particles' locations:

$$\dot{\boldsymbol{x}}_i = -\tau_i \nabla_{\boldsymbol{x}_i} \mathcal{T}_c = -\tau_i \int_{\mathscr{L}_i} \nabla_{\boldsymbol{x}_i} c(\boldsymbol{x}, \boldsymbol{x}_i) \mathrm{d}\boldsymbol{x}, \tag{2}$$

where $\tau_i \geq 0$ is an arbitrary gradient step. In fluid mechanics [13, 16, 4], this is the analog of an *incompressibility force* exerted on each microscopic fluid element. In the present context, this motion leads to repulsion interactions between the particles. Other forces or noise terms can be added in (2), leading to general first-order (stochastic) differential equations systems on the set of positions $\boldsymbol{x}_i$.

3. Main results

Particles with arbitrary shapes can be realized in our framework by considering appropriate cost functions. For instance, in dimension 2, any shape defined by a polar equation $r = r_0(\theta)$ can be encoded by the cost

$$c(\boldsymbol{x}, \boldsymbol{x}_i) = \left(\frac{|\boldsymbol{x} - \boldsymbol{x}_i|}{r_0(\theta(\boldsymbol{x}, \boldsymbol{x}_i))} \right)^{\alpha}.$$

Here, the exponent α plays the role of a deformability (or softness) parameter which dictates the penalty for a particle to deform from its base shape.

This model is already sufficient to generate complex 2D tissues (Fig. 2(a)) and polycrystalline materials [2]. Then one can extend the base dynamics given by (2) by incorporating active forces or random noise to model deformable active particles (Fig. 2(b)). As a canonical example, one simulates deformable Active Brownian Particles (ABP) analogously to [20] to illustrate how volume exclusion and active forces affect fluidity and jamming (Fig. 2(c)). Compared to other computational models, it should be noted that our intrinsically point-particle formulation fits well into a mean-field setting [9] which allows the (formal) derivation of coarse-grained Partial Differential Equations. In the present case, the deformable ABP model leads to the following equation for the density of particles $f(\boldsymbol{x}, \boldsymbol{n})$ at a position $\boldsymbol{x}$ and with the orientation $\boldsymbol{n}$

$$\begin{aligned} &\partial_t f(\boldsymbol{x}, \boldsymbol{n}) + c_0 \nabla_{\boldsymbol{x}} f = \tau \nabla_{\boldsymbol{x}} \cdot (\nabla_{\boldsymbol{x}} \Phi f) + D \Delta_{\boldsymbol{n}} f, \\ &\det \left(\mathrm{I} - \nabla^2_{\boldsymbol{x}} \ell^*(\nabla_{\boldsymbol{x}} \Phi) \nabla^2_{\boldsymbol{x}} \Phi \right) = f. \end{aligned}$$

The potential $\Phi(\boldsymbol{x})$ is the solution of a nonlinear Monge-Ampère equation, which is known in other contexts in physics. The function ℓ^* is the Legendre transform of the function $\ell(\boldsymbol{x}) = |\boldsymbol{x}|^{\alpha}$.

As a more refined model, we propose to incorporate surface tension effects using the cost and force terms

$$c(\boldsymbol{x}, \boldsymbol{x}_i) = \frac{\gamma_{i0}}{R_i} |\boldsymbol{x} - \boldsymbol{x}_i|^2, \quad \boldsymbol{F}_{i \leftarrow j} = \int_{\Gamma_{ij}} \left(\gamma_{ij} |\kappa| + \frac{\eta_{ij}}{|\boldsymbol{x}_i - \boldsymbol{x}_j|} \right) \vec{\boldsymbol{n}} \, \mathrm{d}\sigma.$$

The force $\boldsymbol{F}_{i \leftarrow j}$ exerted on $\boldsymbol{x}_i$ results from elementary pressure-like interactions depending on the local mean curvature κ along each interface $\Gamma_{ij} = \mathscr{L}_i \cap \mathscr{L}_j$ between the Laguerre cells i and j, computed in the direction of the inward normal of $\mathscr{L}_i$. By moving the centroid $\boldsymbol{x}_i$ away from its interface, the first term reduces the local curvature while the second reduces the interface area. The parameters $\gamma_{ij}, \eta_{ij} > 0$ have the dimension of surface tensions. This model satisfies the Young-Dupré relationship for a two-bubble system. More generally it contains all cell sorting phenomena that are commonly used as standardized test cases in computational biology since the work of Chen and Brodland on the so-called Differential Interfacial Tension Hypothesis (DITH) [5]. While most models in the literature are intrinsically 2D, we showcase the applicability of our approach in a fully 3D setting (Fig. 2(d)).

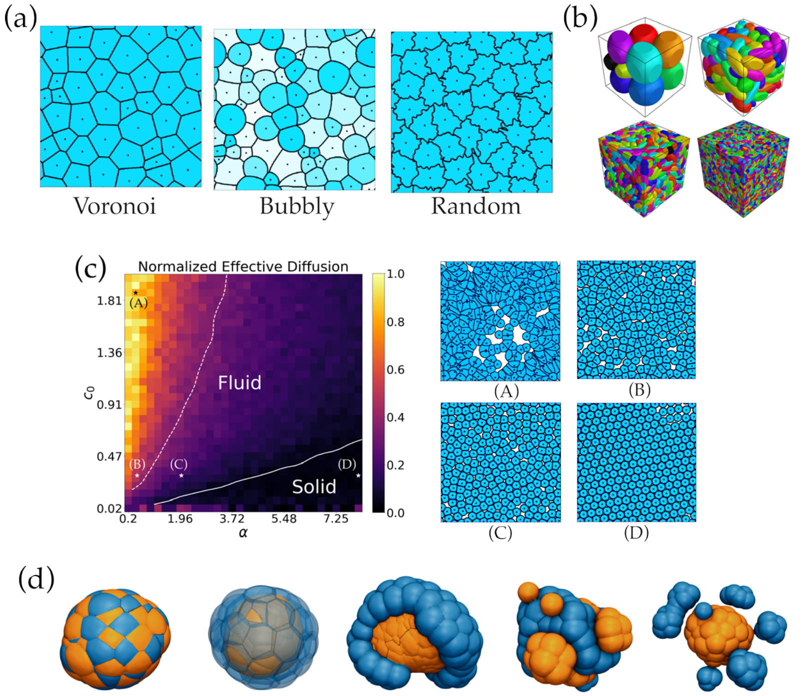

Figure 2. **Main results.** (a) 2D materials with straight, curved or random boundaries. (b) Elongated particles in a box. The model scales from ten to several thousands of particles in 3D. (c) A system of Active Brownian Particles showing a transition from a solid state (hexagonal packing of hard-spheres) to a fluid state (point particles with no shape constraint) depending on the parameter α. (d) Sorting patterns in 3D for two cell types with different surface tension parameters. From left to right: checkerboard, total and partial engulfment, sorting and separation.

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

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Conductive Polymer Composites (CPCs) are widely used in various technological applications. They combine filler conductivity with polymer flexibility. Experimental evidence [1] suggests that critical volume fractions range from 5.5% for small spheres (radius of $1\,\mu$m) to 28% for large spheres (radius of the order of $100\,\mu$m).

In this talk, we present a new off-lattice continuum percolation model that aims to explain the variation in the percolation threshold for different polymers and fillers. Our model comprises a contact algorithm and an aggregation algorithm. The contact algorithm starts with a random arrangement and generates non-overlapping spheres that are at most in contact. The aggregation algorithm produces giant connected components critical for the system's percolative paths. Our approach results in low-volume fraction clusters that are more similar to experimental ones and exhibit similar statistical properties.

CPCs, or conductive polymer composites, exhibit a significant positive temperature coefficient (PTC). This means that as the temperature rises, the polymer expands, causing a separation between the fillers. Consequently, this leads to transitioning from an electrical conductor to an insulator. The specific change depends on the distribution of polymer strain and the bond strength between the filler and the polymer. To investigate this phenomenon, we employ a mesh-free numerical method [2] to solve the 3D thermoelastic equations. Additionally, we analyze the resulting electrical conductivity and calculate the resistivity curve for different thermal strains, which closely resemble experimental results.

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

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Nowadays, hydrogen is mainly produced using fossil fuels. Therefore, clean technologies are necessary to solve this issue. Photocatalysis is a clean technology for hydrogen production and CO_2 conversion. However, its efficiency is limited by the utilized catalyst, which requires high light absorbance, appropriate band structure, and abundant active sites. High-entropy oxides (HEOs) have recently shown great potential as photocatalysts since 2020 [1]. Combining five or more cations gives these materials tunable composition and properties. The large number of elements increases the entropy, stabilizing them in a single or dual crystal structure. In addition, the complex mixture leads to novel photocatalytic properties due to the cocktail effect [1]. Despite of their popularity, few studies are clarifying the effect of electronic structures and differences with conventional photocatalysts.

The current investigation aimed to clarify the characteristics of the band structure and active sites of the first high-entropy photocatalyst, $TiZrHfNbTaO_{11}$, using theoretical calculations and experiments. The synthesis of this sample started with the mixture of metallic powders using a high-pressure torsion method followed by oxidation at 1373 K for 24 h. Subsequently, the crystal structure, optical properties, and photocatalytic activity were examined. Using crystallographic information, the two phases found were modeled using special quasi-random structures (SQS). The powder diffraction patterns were compared with the experimental XRD profiles and further optimized. The electronic structure and active sites were studied in detail using density functional theory calculations performed using the Vienna Ab-Initio Simulation Package (VASP).

Results indicated that the HEO has a band gap comparable to famous photocatalysts such as TiO_2. However, the mixture of elements provides infinite active sites. Our study shows that water adsorption in different sites demonstrates that cations with lower electronegativity, such as Hf and Zr, provide stronger adsorption sites (Fig, 1). In addition, highly electronegative cations enhance the change transfer to the water molecules, improving efficiency. This finding suggests a novel strategy to design efficient high-entropy photocatalysts incorporating cations with different electronegativities [2].

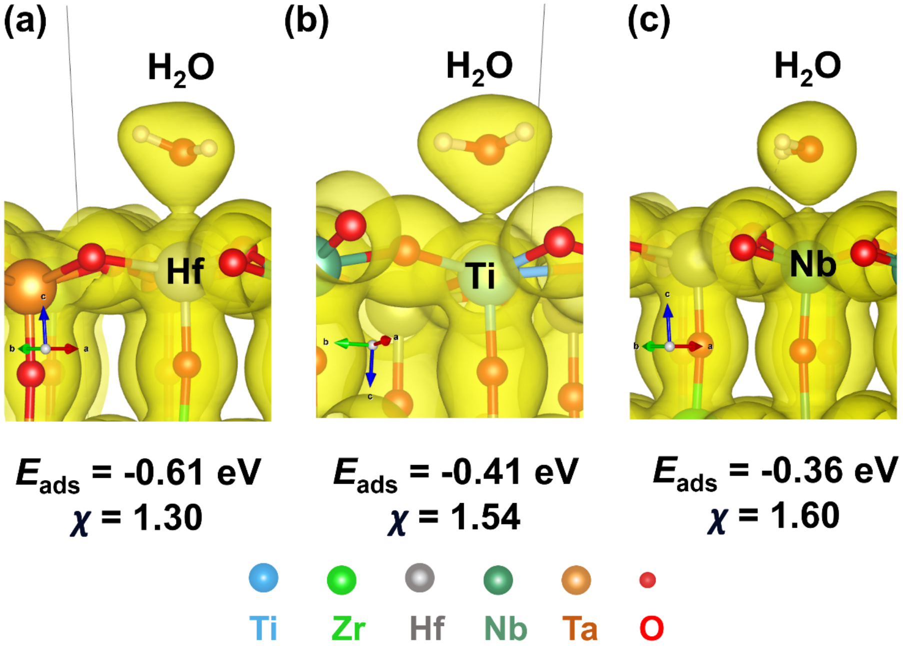

Fig. 1. Charge distribution between the surface of the monoclinic phase of $TiZrHfNbTaO_{11}$ and the water molecule placed on (a) hafnium, (b) titanium, and (c) niobium. E_{ads} refers to the adsorption energy, and χ to the electronegativity.

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Modelling, Analysis, and Finite Element Simulations of Kinematically Incompatible Föppl-von von Krmn Plates

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(joint work with Pierluigi Cesana and Andrs Len Baldelli)

Wedge disclinations play a fundamental role in determining the mechanical behavior of two-dimensional materials like graphene, and their continuum-level description allows for predictive modeling of stress and deformation patterns around these defects. We present both analytical and numerical results for kinematically incompatible Föppl–von Kármán (FvK) plates [1] able to model, within the continuum framework, graphene membranes in presence of defects.

Assuming the plate is free of in-plane tractions and clamped in the out-of-plane direction, we rigorously prove in [2] the existence and regularity of solutions by extending the work of Ciarlet [3], originally developed for kinematically compatible plates. Furthermore, building upon the formulation in [4], we introduce a fully variational Interior Penalty C^0-Discontinuous Galerkin (IPCDG) formulation, identify the key dimensionless parameters of the problem, and perform numerical experiments by varying these parameters over appropriate ranges.

In our model, the kinematic incompatibility stems from the presence of *Volterra wedge disclinations* in the underlying crystalline lattice. These defects occur when a wedge-shaped sector of the crystal is either removed (resulting in a positive wedge disclination) or inserted (resulting in a negative wedge disclination), which in turn produces a discontinuity in the angular orientation of the lattice. In the continuum model, their effects are captured by a discrete distribution of Dirac delta measures.

The mathematical formulation of a kinematically incompatible, isotropic FvK plate consists of two coupled, nonlinear, fourth-order elliptic partial differential equations in the two scalar unknowns: the Airy stress potential v and the out-of-plane displacement w. Let $\Omega \subset \mathbb{R}^2$ denote the mid-plane of the plate in its rest configuration, let $N > 0$ be the number of disclinations, $\{y^{(1)}, \dots, y^{(N)}\} \subset \Omega$ their positions, and $s_i \in \mathbb{R}$ the corresponding Frank angles, then the equations we study are:

$$
\begin{cases} D\Delta^2 w = [v, w] + p & \text{in } \Omega, \\ \dfrac{1}{Eh}\Delta^2 v = -\dfrac{1}{2}[w, w] + \vartheta & \text{in } \Omega, \end{cases} \tag{1}
$$

where

$$
\vartheta := \sum_{i=1}^{N} s_i \delta(x - y^{(i)}), \tag{2}
$$

and where Δ^2 and $[\cdot,\cdot]$ denote, respectively, the biharmonic and the MongeAmpère operators. They are defined as

$$\Delta^2 f := \frac{\partial^4 f}{\partial x_1^4} + 2\frac{\partial^4 f}{\partial x_1^2 \partial x_2^2} + \frac{\partial^4 f}{\partial x_2^4} \quad \text{and} \quad [f,g] := \frac{\partial^2 f}{\partial x_1^2}\frac{\partial^2 g}{\partial x_2^2} + \frac{\partial^2 f}{\partial x_2^2}\frac{\partial^2 g}{\partial x_1^2} - 2\frac{\partial^2 f}{\partial x_1 \partial x_2}\frac{\partial^2 g}{\partial x_1 \partial x_2}\,.$$

Here, E is the Young's modulus, h is the plate thickness, and $D := Eh^3/(12(1-\nu^2))$ is the flexural stiffness, with ν representing the Poisson ratio. The function $p : \Omega \to \mathbb{R}$ models an external transverse load.

Using the direct method in the calculus of variations and following the strategy established by Ciarlet [3] for kinematically compatible plates (i.e., plates free of defects), we rigorously prove that, provided $\partial\Omega$ is Lipschitz and $p \in H^{-2}(\Omega)$, there exists at least one pair of functions $(v, w) \in H_0^2(\Omega) \times H_0^2(\Omega)$ that solves Eq. (1). Moreover, we establish the regularity of the solutions under the assumptions that $\partial\Omega \in C^{4,\gamma}$ for $\gamma \in (0,1)$ and $p \in L^k(\Omega)$ for $k \in [1,\infty]$. These existence and regularity results provide a robust mathematical foundation for the numerical approximation of the model, they ensure that problem (1) is well-posed and that the stress field is smooth away from the defects.

By exploiting the energy functional associated with Eq. (1), we extend the IPCDG formulation of [4] and propose a compact IPCDG finite element formulation in which the penalization terms are directly embedded into a new energy functional. In our implementation, the weak IPCDG formulation of the problem naturally emerges from the first variation of this functional.

After identifying the key dimensionless parameters of problem (1), we explore complex configurations of multiple disclinations, where the defects trigger out-of-plane displacements and lead to the formation of wrinkles (Fig. 1).

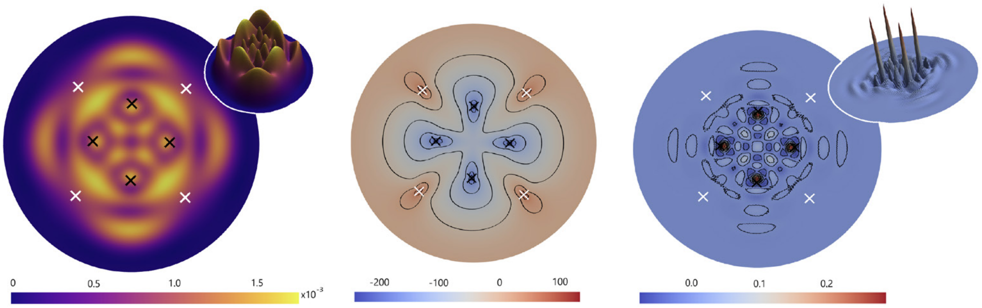

FIGURE 1. LEFT: non-dimensional out-of-plane displacement w. CENTRE: non-dimensional Cauchy stress field in the radial direction σ_{nn}. RIGHT: Gaussian curvature. Black (white) crosses indicate the locations of positive (negative) disclinations.

An immediate application of this study lies in the continuum modeling of graphene sheets containing wedge disclinations in their crystalline lattice.

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

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Computational materials science relies on Kohn-Sham (KS) Density Functional Theory (DFT) [1] to obtain electronic structures and associated level of insight into phenomena, as well as to benchmark force fields and other larger-scale approaches. While the accuracy of KS is often either sufficient (e.g. accuracy of structure optimization) or can we effectively lived with (e.g. bandgap underestimation with GGA functionals) for most applications of computational material science, the formally cubic scaling of KS DFT limits routinely doable calculations to a few hundred atoms and prevents its direct application to intrinsically large-scale phenomena such as microstructure, large interfaces etc. In other words, in many practical applications, it is not the accuracy achievable with DFT exchange-correlation functionals but CPU cost and its scaling that are the bottleneck of achieving more realistic materials modeling.

Methods to address this bottleneck include semiempirical methods, order-N DFT, and orbital-free (OF-) DFT. In this presentation, I will focus on the semiempirical Density Functional Tight Binding (DFTB) [2, 3] method and the ab initio OF-DFT [4] method. DFTB is promising in particular for organic materials and ceramics, for many of which available approximations already provide DFT-like accuracy. With about three orders of magnitude speedup vs. KS-DFT, calculations with $10^{3\text{-}4}$ atoms can be routinely done with DFTB. OF-DFT is already sufficiently accurate for light metal to be used for applied calculations. It is near-linear scaling with small CPU cost prefactors, enabling routine abb initio calculations with 10^6 atoms and beyond.

Both methods, however, suffer from limitations on the range of applicability. DFTB requires parameter sets for all pairs of atoms, and sufficiently accurate DFTB parameters are still not available for many materials. OF-DFT requires a kinetic energy functional (KEF), and sufficiently accurate KEFs (that would allow their use in applications instead of KS DFT) are not available for most materials.

I will present recent efforts in our laboratory in improving the accuracy and extension of the range of applicability of DFTB and OF-DFT with the help of machine learning. For DFTB, I will introduce a DFTB - molecular mechanics hybrid method (DFTB-MM), whereby interatomic Slater-Koster parameters for some pairs of atoms (e.g. unavailable parameters) are replaced with interatomic potentials, whose functional form can be machine-learned [5]. I will show that when interatomic interactions modeled at the MM level do not significantly affect key mechanistic details of the electronic structure, the substitution with a MM potential allows obtaining correct structures, electronic structures, as well as electronic excitation spectra [6], opening way for larger (than doable with KS DFT) scale calculations on materials where existing parameterizations may not be sufficiently accurate (Figure 1).

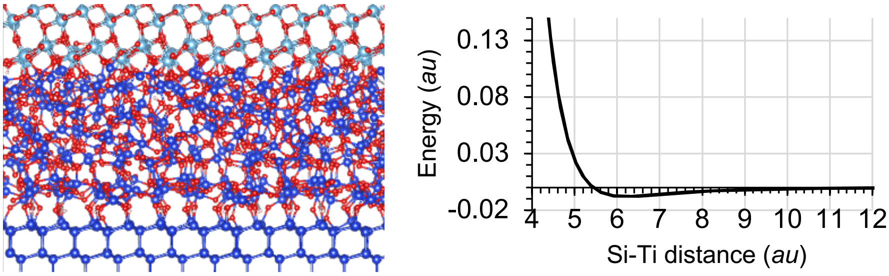

Figure 1. Left: zoom-in on a silicon-silica-titania interface (relevant for silicon-perovskite tandem solar cells) that requires electronic structure-level modeling on the scale of at least 10^3 atoms which was facilitated by the use of DFTB-MM with Ti-Si interactions modeled with a machine-learned potential. Right: the Ti-Si interatomic potential curve.

For OF-DFT, I will show that machine-learning of a KEF requires extremely high ML accuracy, exemplified by correlation coefficients between reference values (computed with KS DFT) and model-predicted values that need to be as high as 0.99999 ("five nines") – much beyond levels of accuracy required in other ML applications such as materials informatics or ML force fields. I will show that such accuracy is in fact obtainable. I will highlight issues related with extremely uneven data distributions faced in this application [7, 8]. I will present examples of machine learning of (space-dependent) kinetic energy densities (KED) [7, 8, 9] as well as kinetic energies [10], ultimately arriving at a machine-learned KEF that is able to reproduce energy-volume curves of hundreds of materials [11] (Figure 2).

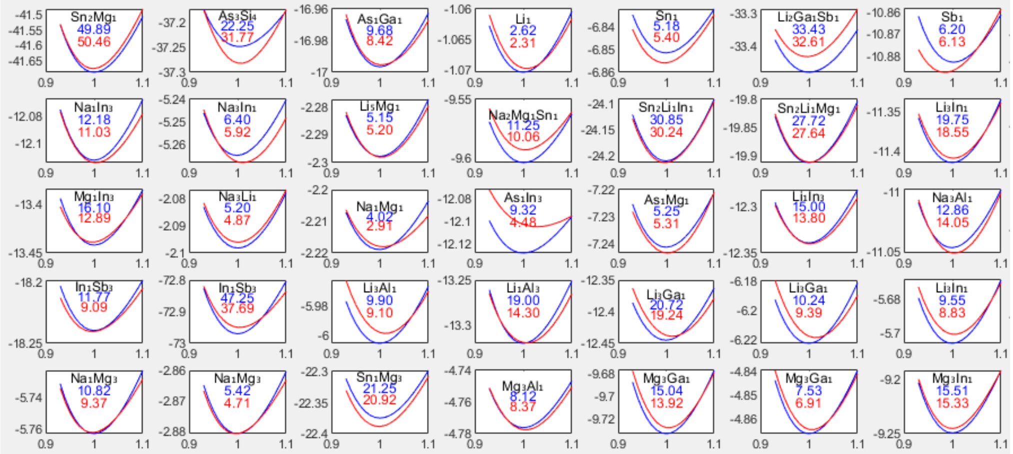

Figure 2. Examples of energy-volume curves of materials obtained with a machine-learned kinetic energy functional (red curved) compared to KS DFT reference (blue curves). Corresponding values of the curvature at the equilibrium geometry are also given ($V_0^2 \frac{d^2E}{dV^2}$ where V_0 is the equilibrium volume).

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[11] https://github.com/sergeimanzhos/GPRKE

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

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Abstract

Cellulose forms highly crystalline fibers by assembling the molecular chains due to strong molecular interactions. Its poor processing performance is an issue since water or general organic solvents cannot dissolve the cellulose fibers. The objective of this study is to gain a deep insight into the dissolution mechanism by elucidating the dissolution state at the microscopic level. Extending the relationship between the number of hydrogen bonds and the solubility in a previous study[1)], we attempted to design solvents with high cellulose dissolving power by integrating high-throughput molecular dynamics (MD) simulation and machine learning (ML). The ML model was used for generating 3,000 chemical structures of imidazolium-based ionic liquids to improve the solubility. Furthermore, the interaction free energy between cation and anion in ionic liquids was found as the metric to characterize cellulose solubility.

Introduction

Cellulose is a highly crystalline fiber composed of molecular chains assembled by complex and strong intermolecular interactions, which makes it insoluble in water and common organic solvents and makes it difficult to process for industrial usage. The objective of this study is to deepen the dissolution mechanism of cellulose by analyzing the dissolution state at the microscopic level. Extending the relationship between the amount of intermolecular hydrogen bonding and solubility based on molecular dynamics (MD) calculations[1,2)], we attempted to design solvents with high solubility.

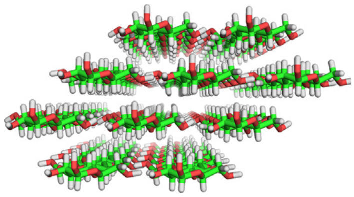

Figure 1. Projection of the *ab* base-plane of cellulose Iβ crystal model (10-chain × 10-mer)

Methods

A crystal model of a cellulose fiber fragment was constructed from the crystal structure data of cellulose Iβ type[3)] (Figure 1). MD calculations were performed under the conditions of constant temperature (400 K), constant pressure (1 bar), and time (250 ns) for the system with an imidazolium-type ionic liquid surrounding the crystal model, using AMBER22 software.

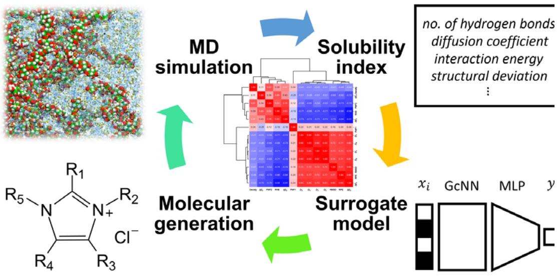

Figure 2. High-throughput MD simulation and ML prediction cycle
Starting from MD simulation, the solubility indexes were calculated. Then, molecular generation was performed based on learned surrogate models.

The modified GAFF was applied to the ionic liquid force field parameters. A graph convolutional neural network (GcNN) model using PyTorch geometric[4)] was constructed. In addition, a reverse analysis using a genetic algorithm by EvoMol[5)] was performed to enumerate the compounds that decrease HB (number of hydrogen bond between cellulose). The anions constituting the ionic liquids were set as chloride ions, and the chemical structures of the cations were modified.

Results and Discussion

We positioned the solubility prediction by MD calculation in the previous studies[1,2)] as a fundamental calculation technique, created predictive models for those calculations, and performed a reverse analysis to see what kind of candidate materials could be obtained if the MD calculation itself was accelerated. The cycle shown in Fig. 2 can be repeated for a wider range of screening faster than the MD search alone, and about 3,000 chemical structures were obtained. The coefficient of determination (R2) for HB was 0.64. As shown in Fig. 3-(a), the prediction accuracy decreased when HB was less than 50% and did not improve throughout the cycle. The free energy change of cation-anion interaction (PMF1) and cellulose-anion interaction (PMF2) were calculated from the radial distribution function as quantities related to HB. The R2 values were 0.92 (PMF1) and 0.88 (PMF2) (Fig. 3-(b), (c)). As shown in Figure 4, HB was also found to be strongly related to the self-diffusion coefficients (D) of PMF1, PMF2, and anions. In particular, the extreme decrease in HB (increase in solubility) and the simultaneous increase in D at certain values of PMF1 can be interpreted as the existence of a threshold for efficient dissociation of the cations and anions of the ionic liquid to function as a cellulose solvent. In particular, the lower PMF2 and cellulose-anion interaction energy change (stronger interaction), the lower HB (increased solubility), which can be interpreted because of the dissolution mechanism by cellulose-anion interaction presented in the previous study[1)].

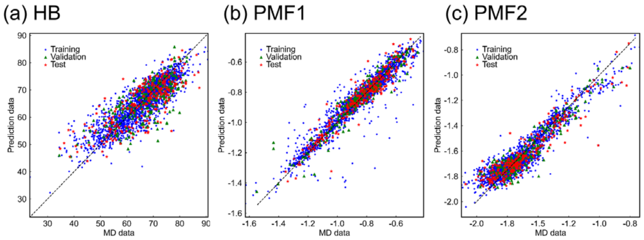

Figure 3. Prediction error plot of HB, PMF1 and PMF2 predictors
(a), (b) and (c) are prediction error plots of HB, PMF1 and PMF2, respectively. The horizon axis indicates the data of MD simulation. The vertical axis indicates the GcNN prediction. The circle, triangle and star shaped points are the data of training, validation, and test, respectively.

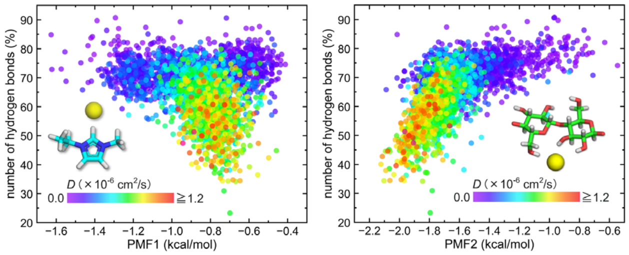

Figure 4. Scatter plot of HB vs. PMF1 and PMF2
The left and right pictures are scatter plots of HB versus PMF1 and PMF2, respectively. The *D* values of diffusion constants (anion) is used for scale bar.

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Machine Learning for Direct Air Carbon Capture: Challenges and Opportunities

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BIO: Dr. P. G. O'Brien is an Associate Professor in the Department of Mechanical Engineering, York University, Canada and has extensive experience working in leading research labs based in materials, mechanical, electrical and chemical engineering. His interdisciplinary research efforts focus on the application of expertise from these fields to develop solutions for a transition to clean energy. Dr. O'Brien has co/authored over fifty journal articles in the areas of materials and energy. His research focuses on the electrification and decarbonization of buildings, energy storage, heat-to-power conversion, and life cycle and techno-economic assessment of energy technologies. He is the founder of the Advanced Materials for Sustainable Energy Technologies Laboratory (AM-SET-Lab) at York University, Canada, where he and his students continue to innovate and advance clean energy solutions.

Abstract: Greenhouse gas (GHG) emissions have raised the Earth's temperature by ~ 1 °C since 1900 and global warming has become an environmental problem of the utmost importance. To tackle global warming world leaders have established the Paris Agreement, which is an international treaty that brings 196 parties together to take action to prevent global temperature increases from exceeding 2 °C [1]. However, GHG emissions and atmospheric carbon dioxide levels continue to rise and have surpassed 420 ppm and are presently more than 50% higher than pre-industrial levels [2]. The global energy-related CO2 emissions were 37.4 gigatonnes (Gt) in 2023 and the rapid deployment of carbon capture technologies is needed to realize the goals established in the Paris agreement [3]. Roadmaps for achieving net zero emissions reported by the IEA estimate that global carbon capture rates must increase to 1.6 GtCO2/y and 7.6 GtCO2/y, by 2030 and 2050, respectively [4].

CO2 capture processes can be classified as point source methods, such as post-combustion, pre-combustion and oxyfuel combustion, or direct air capture (DAC) methods [5-7]. Low- temperature DAC (LT-DAC) processes, which can be deployed at any location, are particularly attractive because the adsorption and desorption phases can occur stepwise in a single unit. Furthermore, LT-DAC processes can be operated at temperatures as low as 100 ° C and can be driven using low-grade thermal energy sources [8]. Nevertheless, further advancements are needed to prove LT-DAC is a viable technology that can be scaled in a cost-effective manner to contribute to achieving net zero emissions on a global scale.

Optimization of DAC processes is highly complicated due to the large number of design parameters and variation in operating environments. Important design choices include the type of adsorbent, the adsorbent bed configuration and operating conditions, input energy sources, and the environment in which the capture system will be deployed [9, 10]. Machine

learning (ML) can provide a great opportunity to improve the performance of DAC systems [11, 12]. However, implementing ML for DAC is challenging considering the broad scope of the key performance indicators, a few of which include: the density, specific surface area, porosity, capacity, of the adsorbent, the geometry of the system and operating conditions such as flow rates, compositions, temperatures and pressures. Furthermore, the acquisition of accurate and reliable data under known conditions presents an even greater challenge.

This work presents examples wherein ML has been used to advance carbon capture processes and discusses the potential for optimizing DAC systems via ML-based approaches. The progress and challenges concerning data acquisition for ML is also presented with an extensive example provided for experimental results from CO2 breakthrough curves [13-15]. This work progresses the development of a data quality framework in support of ML applications for optimizing DAC processes, which can have important implications for achieving widespread, cost-effective, carbon capture at global scales.

Keywords: direct air carbon capture, machine learning, breakthrough curves, negative emission technology.

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Identification and evaluation of promising CO_2 photocapture materials

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(joint work with Victor Eke[1], Kulbir Kaur Ghuman[2], Paul G. O' Brien[1])

Carbon dioxide (CO_2) capture based on the sorption/desorption of gases by solid materials can significantly reduce the energy penalty and equipment costs associated with state-of-the-art CO_2 capture technologies, such as amine scrubbing (*1–6*, *8*). However, these materials suffer from low tolerance to humidity and impurities, low CO_2 adsorption capacities, high capture costs, slow kinetic rates, the requirement of external energy for desorption, and poor CO_2 selectivity. The existing CO_2 sorption/desorption materials either adsorb CO_2 (a) physically, resulting in low selectivity and capacity, or (b) chemically, which, although results in high selectivity and capacity, requires external energy (typically heat generated from fossil fuel combustion) to desorb the strongly adsorbed CO_2 and regenerate the material. Thus, a large barrier to realizing CO_2 sorption/desorption technologies commercially is the lack of the 'ideal' material, which adsorbs CO_2 selectively and readily desorbs CO_2 with minimal energy input when required. In this regard, the development of new methods of capturing CO_2 using materials under external stimuli, such as light irradiation and electric fields, plays a pivotal role in improving the energy efficiency of carbon capture technologies.

This research focuses on the development of solid adsorbents that leverage a photodesorption mechanism to capture CO_2 with remarkably high efficiency (*7*, *8*). These materials readily adsorb CO_2 in the dark or low-illumination environments and subsequently photo-desorb captured CO_2 when exposed to incident light. By utilizing light as a "photoswitch" to trigger CO_2 desorption, the need for energy-intensive pressure or temperature alteration is mitigated. Herein, a combination of computational and experimental methods are employed to develop and validate the photo-driven carbon capture concept. Density Functional Theory (DFT) calculations were utilized to systematically screen a range of metal candidates, identifying those exhibiting favorable CO_2 adsorption characteristics and the potential for efficient photodesorption (*8*).

A custom-built experimental setup capable of measuring CO_2 breakthrough curves under illuminated conditions was carefully designed and assembled to validate the computational predictions. The quantification of CO_2 adsorption capacities and the ability to capture CO_2 using light as a "photoswitch" is assessed. Experiments are conducted for a variety of sorbent materials including pure metal supported on aerogel, amine-functionalized silica, and zeolites. The results demonstrate incident light can facilitate CO_2 capture for some adsorbents, which has important implications for lowering the "energy penalty" associated regenerating adsorbents and for the development of solar-driven CO_2 capture technologies.

Subsequent steps in this research will involve exploring various metal-alloys and mixed-metal oxide systems, with the goal of further enhancing CO_2 adsorption and photodesorption capabilities, as well as optimizing the energy efficiency and overall cost effectiveness of the process. Moreover, a comprehensive Life Cycle Assessment (LCA) to evaluate the environmental and economic feasibility of scaling up these materials for CO_2 capture will be conducted. This study establishes a framework for the continued enhancement and application of light-activated sorbents within scalable carbon capture and regeneration systems.

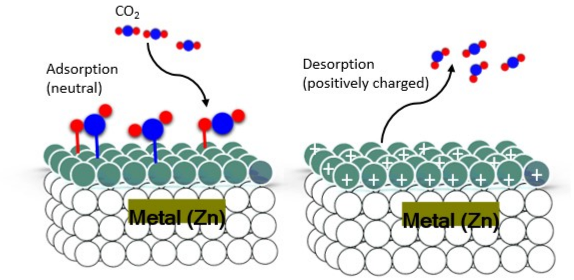

FIGURE 1. CO_2 adsorbing on Zn surface in neutral state and desorbing when the surface is positively charged.

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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

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The urgent need to achieve net-zero emissions by 2050 has intensified interest in Direct Air Carbon Capture and Storage (DACCS) technologies as a crucial negative emissions strategy. While DACCS shows promise for atmospheric carbon dioxide removal, comprehensive understanding of its life cycle environmental impacts across different geographical contexts and system configurations remains limited. Building on prior life cycle assessments (LCA) of DACCS, including the work of Madhu et al., (2021), this study presents a detailed LCA of low-temperature (LT) DACCS systems, examining regional variations in performance and the critical role of energy system integration in determining overall life cycle efficiency.

Our analysis employs a cradle-to-grave LCA approach following ISO 14040 and 14044 standards, utilizing OpenLCA software with the Ecoinvent 3.10 database and ReCiPe Midpoint (H) impact assessment method. We evaluate three distinct DACCS system configurations: (1) grid electricity with natural gas heating, (2) grid electricity with solar thermal heating, and (3) grid electricity with solar thermal and auxiliary electric heating. The study encompasses seven regions with diverse energy profiles: four Canadian provinces (Quebec, Ontario, New Brunswick, Alberta), Switzerland, Greece, and China. This geographical spread allows us to assess how varying grid electricity mix and solar resource availability influence system performance.

The results reveal substantial variations in greenhouse gas (GHG) emissions across configurations and regions. Solar-only systems consistently demonstrate superior performance, with emissions ranging from 79 kg CO_2-eq/tCO_2 captured in Quebec to 366 kg CO_2-eq/tCO_2 in China. The integration of auxiliary heating increases emissions by an average of 253 kg CO_2-eq/tCO_2 across all regions, while natural gas-based systems show the highest emissions, ranging from 283 to 582 kg CO_2-eq/tCO_2. These variations primarily stem from differences in grid carbon intensity and local infrastructure requirements.

Process contribution analysis identifies critical emission sources across system configurations. The solar collector system contributes 3-40% of total emissions in solar-only configurations, with regional variations reflecting differences in manufacturing emissions and installation requirements. Infrastructure accounts for 6-27% of emissions across all configurations, while CO_2 transport and storage processes contribute 15-56% of total emissions, highlighting the importance of existing infrastructure in determining system performance.

Life cycle efficiency calculations demonstrate the superior carbon removal effectiveness of solar-based systems, achieving efficiencies between 92% (Quebec) and 63% (China), compared to 42-72% for natural gas systems. Sensitivity analysis of regeneration energy requirements reveals that for every 1 GJ/tCO_2 increase, emissions rise by approximately 8 kg CO_2-eq/tCO_2 in solar-only systems, 45 kg CO_2-eq/tCO_2 with auxiliary heating, and 168 kg CO_2-eq/tCO_2 in natural gas systems, emphasizing the crucial importance of minimizing regeneration energy requirements.

Our findings have significant implications for DACCS deployment strategies and technology development. The analysis suggests that optimal deployment locations should prioritize both solar resource availability and grid cleanliness, with potential emissions reductions of up to 290 kg CO_2-eq/tCO_2 achievable through careful site selection and system configuration. The substantial efficiency penalties associated with natural gas systems indicate their deployment should be limited to scenarios where solar-based heating is impractical. Our analysis aligns with and expands upon findings from Cooper et al., (2022), Qiu et al., (2022), and Terlouw et al., (2021), reinforcing the importance of renewable energy use in minimizing greenhouse gas emissions and resource trade-offs.

Our comprehensive analysis highlights the importance of adopting a system-level approach (careful system design and siting decisions) to DACCS deployment. While heating system selection remains crucial, the substantial contributions from infrastructure, transport, and storage processes indicate that optimization efforts must address all system components. These insights can inform policy decisions and deployment strategies aimed at maximizing carbon removal efficiency while minimizing environmental impact aligned with global net-zero emissions targets.

Keywords: direct air carbon capture and storage (DACCS), energy system integration, global warming potential (GWP), life cycle assessment (LCA), life cycle efficiency, negative emissions technology (NET), solar thermal energy

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Optimization of Transition Metal Alloy Adsorbents for CO2 Capture Using Machine Learning (ML) and Density Functional Theory (DFT)

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BIO: Yasser Salah Eddine Bouchareb is a data scientist and mathematician specializing in deep learning and computational material science. He is currently a Ph.D. candidate in Energy and Materials Sciences at INRS in Montreal, Canada. His research focuses on accelerating the discovery of materials for carbon capture using machine learning and density functional theory (DFT). Yasser was previously an AI Resident at Google Research, where he worked on deep learning theory and applications. He holds multiple master's degrees in applied mathematics and machine intelligence from AIMS Rwanda, AIMS South Africa, University of Cape Town, and the University of Constantine. His work spans from large-scale satellite-based building detection in Africa to disease classification in crops, and he's an active contributor to the African AI community through events like Deep Learning Indaba.

Abstract: The increasing levels of atmospheric CO2 necessitate the development of effective carbon capture technologies to mitigate climate change. This study explores the optimization of transition metal alloy adsorbents for CO2 capture using a combination of Density Functional Theory (DFT) and Machine Learning (ML). Bimetallic surfaces offer a promising avenue for enhancing adsorption selectivity and efficiency, leveraging ligand and strain effects to improve CO2 affinity. However, the computational cost associated with high-throughput DFT calculations remains a significant bottleneck.

To address this challenge, we integrate ML models to accelerate the prediction of adsorption energies and structural relaxations. We develop a dataset of 75 transition metal alloys, analyzing adsorption characteristics through DFT simulations performed using Quantum ESPRESSO and the Vienna Ab initio Simulation Package (VASP). Machine learning models, including Graph Neural Networks (GNNs) such as DimeNet++, SchNet, and EquiFormerV2, are trained on these datasets to predict adsorption behaviors with reduced computational overhead.

Results demonstrate that ML models can approximate DFT-calculated total energies with a mean absolute error (MAE) of ~0.425 eV, significantly reducing computational time from days to minutes. These findings highlight the potential of ML-driven approaches in accelerating material discovery for carbon capture applications.

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

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Human breath contains over 3000 volatile organic compounds, abnormal concentrations of which can indicate the presence of certain diseases. Recently, metal-organic framework (MOF)-metal oxide composite materials have been explored for chemiresistive sensor applications, however their ability to detect breath compounds associated with specific diseases remains unknown. In this presentation, I will present our new high-throughput computational protocol for evaluating the sensing ability of MOF-metal oxide towards small organic compounds.[1] This protocol uses a cluster-based method for accelerated structure relaxation, and a combination of binding energies and density-of-states analysis to evaluate sensing ability, the latter measured using Wasserstein distances. We apply this protocol to the case of the MOF-metal oxide composite material NM125-TiO_2 and show that it is consistent with previously reported experimental results for this system. We examine the sensing ability of NM125-TiO_2 for over 100 human-breath compounds spanning 13 different diseases. Statistical inference then allows us to identify ones which subsequent experimental efforts should focus on. The work provides new tools for computational sensor research, while also illustrating how computational materials science can be integrated into the field of preventative medicine.

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

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Catalysts are essential for chemical transformations in energy conversion, environmental sustainability, and material synthesis. While early catalyst discovery relied on empirical methods, the development of quantum chemical calculations, particularly density functional theory (DFT) method, has significantly advanced rational catalyst design. However, despite its accuracy, DFT calculations remain computationally expensive, especially for large and complex catalytic systems such as supported metal nanoparticles (NPs). To bypass these computational costs, descriptor-based approaches have been developed to correlate geometrical and electronic properties with catalytic performance. Among these, the *d*-band center model, which represents catalytic activity through a single energy quantity, has proven insufficient, particularly in nanoparticle systems [1-3], where the large number of adsorption sites introduces significant electronic and structural variability.

The electronic structure of materials fundamentally determines their chemical and physical properties. The Density of States (DOS) provides a detailed distribution of electronic states as a function of energy, offering critical insights into catalytic activity. When an adsorbate interacts with a catalyst surface, electron transfer occurs at specific energy levels within the material's DOS, directly influencing adsorption stability, molecular activation, and subsequent reaction pathways. Identifying the specific DOS regions responsible for these interactions is crucial for both fundamental understanding and rational catalyst design. To address this challenge, the Electronic Structure Decomposition Approach (ESDA) was developed as a systematic framework to identify the DOS regions governing catalytic activity [3].

In this study, ESDA is applied to Ru nanoparticles (Ru NPs), key catalysts in Fischer-Tropsch (FT) synthesis, where CO and H_2 are converted into liquid hydrocarbons. While Ru is highly efficient at activating CO, its scarcity and high cost limit its large-scale industrial application. Thus, understanding what makes Ru uniquely effective in CO activation is essential for designing alternative catalysts or optimizing Ru-based systems. Using ESDA, the electronic structure of Ru NPs is decomposed into energy-resolved DOS regions to identify the key electronic features governing CO adsorption and activation.

Within the ESDA framework, the DOS was systematically partitioned into 1 eV-separated energy regions, categorizing them into *s*-, *p*-, e_g-, t_{2g}-, and *d*-states of Ru atoms before CO interaction. Specifically, DOS contributions from Ru atoms at the adsorption site (AS), surface nearest neighbors (sNN), and subsurface nearest neighbors (bNN) within the energy range of −7 to +2 eV were analyzed. These energy-resolved DOS areas served as input descriptors in multiple linear regression models, trained on DFT-calculated CO adsorption energies (E_{ads}) and C–O vibrational frequencies (ν_{CO}), the latter serving as a measure of CO bond activation. Figure 1 illustrates the relationship between DOS contributions of Ru atoms (AS, sNN, bNN) and E_{ads} and ν_{CO}.

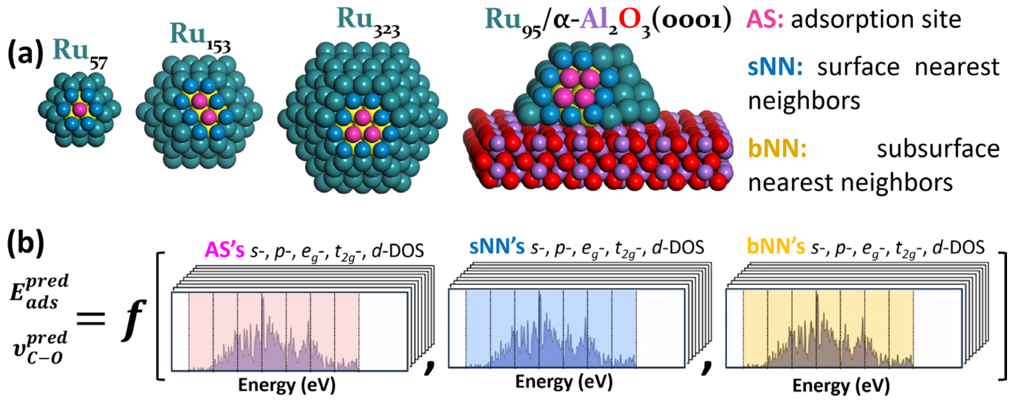

Figure 1. (a) Illustration of isolated and supported Ru NPs, highlighting the Ru atoms at the AS, sNN, and bNN and (b) representation of E_{ads} and ν_{CO} as a linear combination of the DOS contributions from these Ru atoms.

Through this approach, CO adsorption and activation trends across different Ru NPs have been accurately predicted, enabling a transition from electronic structure analysis to catalyst optimization. Figure 2 illustrates the DOS regions governing ν_{CO}.

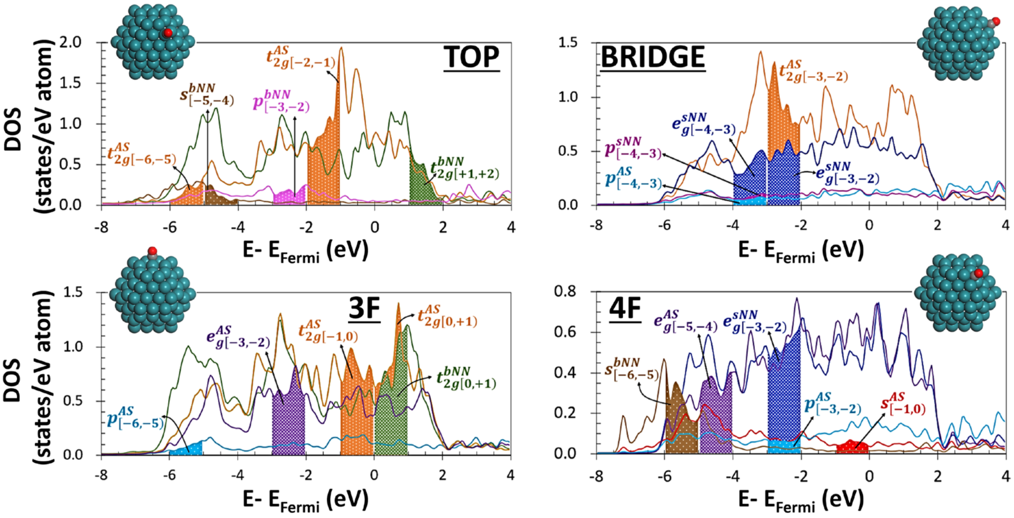

Figure 2. DOS regions governing C–O bond activation upon CO interaction at the top, bridge, threefold (3F), and fourfold (4F) sites of isolated Ru NPs.

Following the identification of the DOS regions responsible for CO activation, catalyst performance was further engineered by modifying the Ru electronic structure. To achieve this, α-Al_2O_3(0001) was introduced as a support material, as it is known to increase Ru dispersion, improve thermal stability, and provide interfacial active sites that enhance catalytic activity. The Ru/Al_2O_3 interface was hypothesized to modify the electronic environment of Ru, potentially promoting CO activation. Using ESDA, the impact of Al_2O_3 is predicted without requiring additional DFT calculations, enabling a rapid and cost-effective analysis of support effects. The results indicate that CO activation is enhanced at the Ru/Al_2O_3 interface, particularly at fourfold (4F) sites, where the C–O bond length increases and the vibrational frequency decreases by 15%, as shown in Figure 3. The redshifted vibrational frequencies indicate a weakened C–O bond, which may correspond to a lower activation energy and facilitated dissociation. This improvement is highly relevant for FT synthesis, where efficient CO dissociation directly enhances hydrocarbon formation.

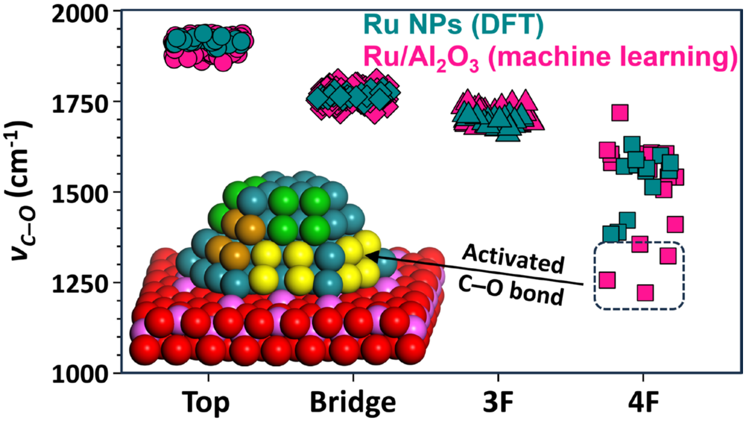

Figure 3. Influence of α-Al_2O_3(0001) on v_{CO} upon CO interaction at the top, bridge, 3F, and 4F sites of Ru NPs

Beyond simply analyzing electronic interactions, ESDA provides a direct strategy for catalyst optimization. Unlike conventional descriptor-based approaches, ESDA enables the precise identification and modification of DOS regions to enhance catalytic performance, offering a quantitative framework for rational catalyst design. Furthermore, pretrained ESDA models eliminate the need for extensive DFT calculations, significantly accelerating catalyst screening and materials discovery. ESDA is 4.8 times more efficient than DFT for predicting the impact of Al_2O_3, and when training data is available, it accelerates prediction speed by up to 22.6 times.

In summary, ESDA has been demonstrated to be not only a powerful analytical tool but also a predictive framework for catalyst engineering. By decoding the electronic structure of Ru NPs and subsequently engineering their catalytic activity via support interactions, a new pathway for rational catalyst design is established. While this study focuses on Ru-based catalysts for FT synthesis, the ESDA methodology is broadly applicable to other catalytic systems. As ESDA continues to evolve, its integration with high-throughput computational screening and data-driven catalyst discovery could transform computational catalysis, accelerating the development of next-generation catalytic materials for sustainable energy and industrial applications.

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

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In this contribution, we address quantum transport in long periodic arrays whose basic cells, localized potentials U(x), display certain particular features. We investigate under which conditions these “local” special characteristics can influence the tunneling behavior through the full structure. As the building blocks, we consider two types of U(x)s: combinations of either P¨oschl–Teller, $U_0/\cosh^2[\alpha x]$, potentials (for which the reflection and transmission coefficients are known analytically) or Gaussian-shaped potentials. For the latter, we employ an improved potential slicing procedure using basic barriers, like rectangular, triangular and trapezoidal, to approximate U(x) and thus obtain its scattering amplitudes. By means of a recently derived method, we discuss scattering along lattices composed of a number, N, of these U(x)s. We find that near-resonance energies of an isolated U(x) do impact the corresponding energy bands in the limit of very large Ns, but only when the cell is spatially asymmetric. Then, there is a very narrow opening (defect or rip) in the system conduction quasi band, corresponding to the energy of the U(x) quasi-state. Also, for specific U_0’s of a single P¨oschl–Teller well, one has 100% transmission for any incident $E > 0$. For the U(x) parameters rather close to such a condition, the associated array leads to a kind of “reflection comb” for large Ns; $|T_N(k)|^2$is not close to one only at very specific values of k, when $|T_N|^2 \approx 0$. Finally, the examples here (see Fig. 1) — illustrating how the anomalous transport comportment in finite but long lattices can be inherited from certain singular aspects of the U(x)s — are briefly discussed in the context of known effects in the literature, notably for lattices with asymmetric cells.

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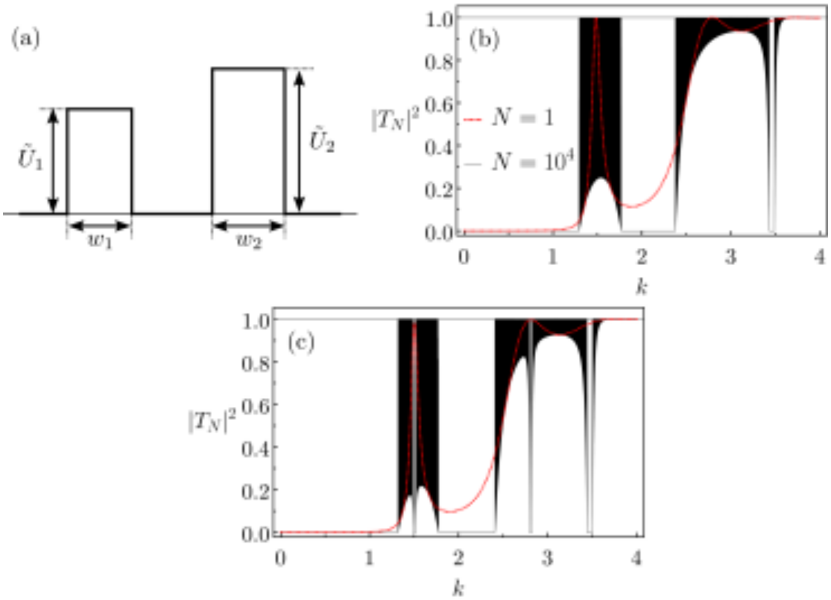

Figure 1. (a) Illustration of a building block formed by two rectangular barriers, with widths w_1, w_2 and heights $\tilde{U}_1$, $\tilde{U}_2$. Graph of the transmission probability in terms of the wavenumber k, when we consider (b) a symmetrical and (c) an asymmetrical cell. In (b) $\tilde{U}_2 = 2$, and in (c) $\tilde{U}_1 = 2.2$. The remain parameters are $w_1 = w_2 = 1$, $\tilde{U}_1 = 2$ in both figures. The width between any two consecutive barriers is unitary.

Variational analysis of elastoplastic deformation of structured materials

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Structured materials, such as metallic alloys with atomic-scale layers, show peculiar deformation patterns, which may have significant implications on material properties. In this presentation, we discuss one possible approach to modeling and understanding of this kind of pattern formation through the so-called rate-independent evolution in the variational setting of finite-strain crystal elasto-plasticity [4].

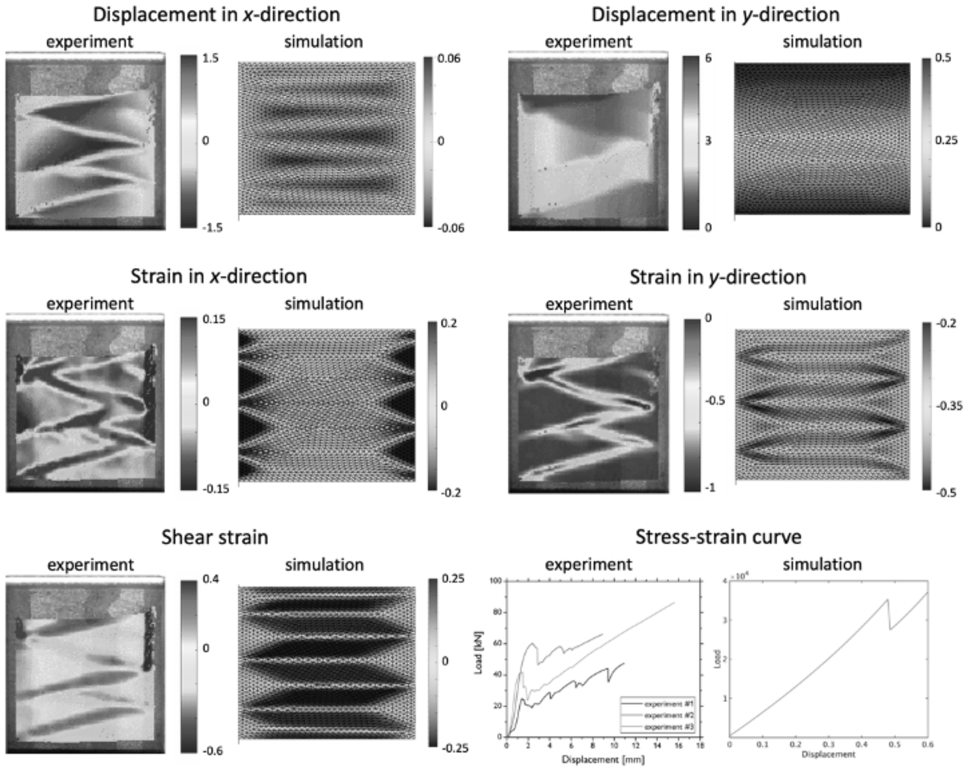

Figure 1: Comparison of numerical simulations and experimental results for the compression of a stack of papers.

We start with a mathematical analysis of the macroscopic behavior of mille-feuille structured crystalline materials, which is composed by alternating rigid and soft layers. This is done within the mathematical framework of homogenization via Γ-convergence. We present a generalization of a result by Christowiak and Kreisbeck [1], where more than one slip system is active in the soft layers [3]. This analysis provides an explicit formula for the homogenized energy.

Next, we build a mathematical model of an evolutionary rate-independent system, which reflects the theoretically obtained insights, and study its mathematical properties. We perform numerical simulations of this mathematical model using a finite element approximation and an inbuilt Matlab minimization function. Finally, we have carried out an experiment compressing a stack of papers and investigated the resulting deformation using digital image correlation analysis. It turned out that the results of numerical simulations are in a very good agreement with experimental measurements [2]. We report on these numerical and experimental studies, commenting on unresolved tasks and future research directions.

This is joint work with D. Drozdenko, M. Knapek, M. Kružík, K. Máthis and J. Valdman (Prague) and A. Ishikawa (Kyoto).

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Designing long-life shape memory alloys using the triplet condition

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Shape memory alloys exhibit unique properties, including the shape memory effect, where deformation is reversed upon heating, and superelasticity, characterized by rubber-like behavior. These properties, driven by thermoelastic martensitic transformation between high-symmetry austenite and low-symmetry martensite phases, enable diverse applications such as medical devices, actuators, and solid-state refrigeration. However, their use is limited by functional fatigue, including transformation temperature changes and reduced strain, caused by dislocation accumulation during transformation. This issue arises from incompatibilities in martensitic microstructures.

We propose a novel geometrical criterion for achieving highly compatible martensitic microstructures and elaborate on its mechanism. Addressing functional fatigue in shape memory alloys, particularly enhancing thermal cycling stability, has been a persistent challenge in the field. Ensuring martensitic compatibility provides a groundbreaking approach to alloy design. The cofactor condition (CC) [1] serves as a geometrical framework to simultaneously resolve incompatibilities at parent/martensite and martensite/martensite interfaces. However, satisfying CC often imposes strict constraints on alloy composition.

In our work, we identify an alternative condition that enables the emergence of unique martensitic microstructures, mimicking the effects of CC without requiring its stringent constraints. This condition, termed the triplet condition (TC)[2], offers a new pathway for designing supercompatible martensite structures. Unlike CC, which is fulfilled along curves in the eigenvalue space of lattice deformation, TC is satisfied across two-dimensional surfaces, making it significantly easier to meet. We also present detailed findings on the martensitic microstructures and dislocation behavior observed in Ti-Ni-based alloys that closely adhere to TC.

Let $\mathbf{U}$, $\mathbf{V}$, $\mathbf{W} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}+}$ be the deformation gradients of martensitic variants that are mutually in a twin relationship, and assume $\mathbf{R}_{\mathrm{vw}}\mathbf{W} = \mathbf{V} + \mathbf{b} \otimes \mathbf{m}$ for some $\mathbf{R}_{\mathrm{vw}} \in SO(3)$, $\mathbf{b}$, $\mathbf{m} \in \mathbb{R}^3$. Then, the three variants can form compatible triple junction if and only if

$$(\mathbf{V}\mathbf{b})^{T}\mathrm{cof}(\mathbf{V}^2 - \mathbf{U}^2)\mathbf{m} = 0$$
$$\mathrm{tr}\,(\mathbf{U}^{-1}\mathbf{V}^{2}\mathbf{U}^{-1}) - |\mathbf{b}|^2|\mathbf{U}^{-1}\mathbf{m}|^2/4 \geq 3$$

hold. This condition is known as the triplet condition [2]. The expression of this condition using the eigenvalues of the cubic-to-orthorhombic transformation (α, β, γ) in Ti-Ni-based alloys is as follows.

$$\alpha^2\gamma^2 + 2\gamma^2\beta^2 - 3\alpha^2\beta^2 = 0 \quad \text{(TC I)}$$
$$2\alpha^2 + \beta^2 - 3\gamma^2 = 0 \quad \text{(TC II)}$$

The triple junction formed by the three variants joined through type I twinning is referred to as TC I, while the triple junction formed through type II twinning is referred to as TC II. For more details, refer to the reference [2].

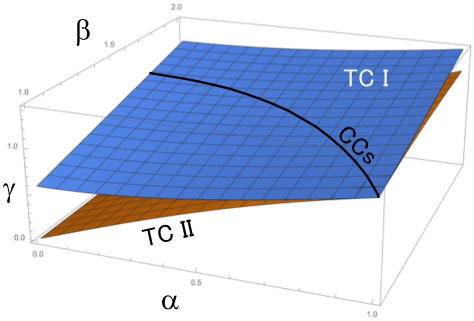

Figure 1. Parametric surfaces of TCI and TC II

Figure 1 shows the parametric surfaces of TCI and TCII in the eigenvalue space. By adjusting the alloying elements to align the eigenvalues of **U** along these surfaces, alloys satisfying the triplet condition can be obtained. The curve representing the CCs are also depicted in Fig. 1. It is evident that satisfying the TC is much easier. Ti-Ni-Cu [3] nearly satisfies the triplet condition and exhibits a unique microstructure, as shown in Figure 2, composed solely of twinning interfaces. When this microstructure forms, the accumulation of dislocations during repeated transformations is dramatically suppressed [4]. In the presentation, we will discuss in detail the microstructures of alloys satisfying the TC, their formation process, and their shape memory properties, demonstrating that the TC is a useful design guideline for developing long-life shape memory alloys.

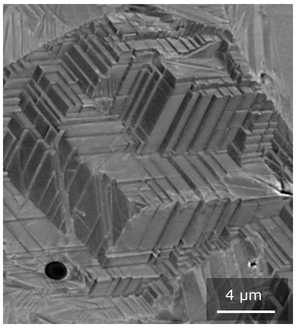

Figure 2. Peculiar martensite microstructure in Ti-30Ni-20Cu

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MI レクチャーノートシリーズ刊行にあたり

本レクチャーノートシリーズは、文部科学省 21 世紀 COE プログラム「機能数理学の構築と展開」（H15-19 年度）において作成した COE Lecture Notes の続刊であり、文部科学省大学院教育改革支援プログラム「産業界が求める数学博士と新修士養成」（H19-21 年度）および、同グローバル COE プログラム「マス・フォア・インダストリ教育研究拠点」（H20-24 年度）において行われた講義の講義録として出版されてきた。平成 23 年 4 月のマス・フォア・インダストリ研究所（IMI）設立と平成 25 年 4 月の IMI の文部科学省共同利用・共同研究拠点として「産業数学の先進的･基礎的共同研究拠点」の認定を受け、今後、レクチャーノートは、マス・フォア・インダストリに関わる国内外の研究者による講義の講義録、会議録等として出版し、マス・フォア・インダストリの本格的な展開に資するものとする。

2022 年 10 月
マス・フォア・インダストリ研究所
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MI Lecture Note Vol.77	松谷　茂樹 佐伯　修 中川　淳一 田上　大助 上坂　正晃 Pierluigi Cesana 濵田　裕康	平成29年度　九州大学マス・フォア・インダストリ研究所 共同利用研究集会（I） 結晶の界面，転位，構造の数理　148pages	December 20, 2017
MI Lecture Note Vol.78	瀧澤　重志 小林　和博 佐藤憲一郎 斎藤　努 清水　正明 間瀬　正啓 藤澤　克樹 神山　直之	平成29年度　九州大学マス・フォア・インダストリ研究所 プロジェクト研究　研究集会（I） 防災・避難計画の数理モデルの高度化と社会実装へ向けて 136pages	February 26, 2018
MI Lecture Note Vol.79	神山　直之 畔上　秀幸	平成29年度　AIMaP チュートリアル 最適化理論の基礎と応用　96pages	February 28, 2018
MI Lecture Note Vol.80	Kirill Morozov Hiroaki Anada Yuji Suga	IMI Workshop of the Joint Research Projects Cryptographic Technologies for Securing Network Storage and Their Mathematical Modeling　116pages	March 30, 2018
MI Lecture Note Vol.81	Tsuyoshi Takagi Masato Wakayama Keisuke Tanaka Noboru Kunihiro Kazufumi Kimoto Yasuhiko Ikematsu	IMI Workshop of the Joint Research Projects International Symposium on Mathematics, Quantum Theory, and Cryptography　246pages	September 25, 2019
MI Lecture Note Vol.82	池森　俊文	令和２年度　AIMaP チュートリアル 新型コロナウイルス感染症にかかわる諸問題の数理 145pages	March 22, 2021

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MI Lecture Note Vol.83	早川健太郎 軸丸　芳揮 横須賀洋平 可香谷　隆 林　　和希 堺　　雄亮	シェル理論・膜理論への微分幾何学からのアプローチと その建築曲面設計への応用　49pages	July 28, 2021
MI Lecture Note Vol.84	Taketoshi Kawabe Yoshihiro Mizoguchi Junichi Kako Masakazu Mukai Yuji Yasui	SICE-JSAE-AIMaP Tutorial Advanced Automotive Control and Mathematics　110pages	December 27, 2021
MI Lecture Note Vol.85	Hiroaki Anada Yasuhiko Ikematsu Koji Nuida Satsuya Ohata Yuntao Wang	IMI Workshop of the Joint Usage Research Projects Exploring Mathematical and Practical Principles of Secure Computation and Secret Sharing　114pages	February 9, 2022
MI Lecture Note Vol.86	濱田　直希 穴井　宏和 梅田　裕平 千葉　一永 佐藤　寛之 能島　裕介 加葉田雄太朗 一木　俊助 早野　健太 佐伯　　修	2020年度採択分　九州大学マス・フォア・インダストリ研究所 共同利用研究集会 進化計算の数理　135pages	February 22, 2022
MI Lecture Note Vol.87	Osamu Saeki, Ho Tu Bao, Shizuo Kaji, Kenji Kajiwara, Nguyen Ha Nam, Ta Hai Tung, Melanie Roberts, Masato Wakayama, Le Minh Ha, Philip Broadbridge	Proceedings of Forum “Math-for-Industry” 2021 -Mathematics for Digital Economy-　122pages	March 28, 2022
MI Lecture Note Vol.88	Daniel PACKWOOD Pierluigi CESANA, Shigenori FUJIKAWA, Yasuhide FUKUMOTO, Petros SOFRONIS, Alex STAYKOV	Perspectives on Artificial Intelligence and Machine Learning in Materials Science, February 4-6, 2022　74pages	November 8, 2022

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MI Lecture Note Vol.89	松谷　茂樹 落合　啓之 井上　和俊 小磯　深幸 佐伯　　修 白井　朋之 垂水　竜一 内藤　久資 中川　淳一 濵田　裕康 松江　　要 加葉田雄太朗	2022年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 材料科学における幾何と代数 III　356pages	December 7, 2022
MI Lecture Note Vol.90	中山　尚子 谷川　拓司 品野　勇治 近藤　正章 石原　　亨 鍛冶　静雄 藤澤　克樹	2022年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 データ格付けサービス実現のための数理基盤の構築　58pages	December 12, 2022
MI Lecture Note Vol.91	Katsuki Fujisawa Shizuo Kaji Toru Ishihara Masaaki Kondo Yuji Shinano Takuji Tanigawa Naoko Nakayama	IMI Workshop of the Joint Usage Research Projects Construction of Mathematical Basis for Realizing Data Rating Service 610pages	December 27, 2022
MI Lecture Note Vol.92	丹田　　聡 三宮　　俊 廣島　文生	2022年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 時間・量子測定・準古典近似の理論と実験 ～古典論と量子論の境界～　150pages	Janualy 6, 2023
MI Lecture Note Vol.93	Philip Broadbridge Luke Bennetts Melanie Roberts Kenji Kajiwara	Proceedings of Forum “Math-for-Industry” 2022 -Mathematics of Public Health and Sustainability-　170pages	June 19, 2023
MI Lecture Note Vol.94	國廣　　昇 池松　泰彦 伊豆　哲也 穴田　啓晃 縫田　光司	2023年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 現代暗号に対する安全性解析・攻撃の数理　260pages	Janualy 11, 2024
MI Lecture Note Vol.96	澤田　茉伊	2023年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 デジタル化時代に求められる斜面防災の思考法　70pages	March 18, 2024

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MI Lecture Note Vol.97	Shariffah Suhaila Syed Jamaludin Zaiton Mat Isa Nur Arina Bazilah Aziz Taufiq Khairi Ahmad Khairuddin Shaymaa M.H.Darwish Ahmad Razin Zainal Abidin Norhaiza Ahmad Zainal Abdul Aziz Hang See Pheng Mohd Ali Khameini Ahmad	International Project Research-Workshop (I) Proceedings of 4th Malaysia Mathematics in Industry Study Group (MMISG2023)　172pages	March 28, 2024
MI Lecture Note Vol.98	中澤　嵩	2024年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 自動車性能の飛躍的向上を目指すData-Driven設計　92pages	January 30, 2025
MI Lecture Note Vol.99	Jacques Garrigue	2024年度採択分 九州大学マス・フォア・インダストリ研究所 共同利用研究集会 コンピュータによる定理証明支援とその応用　308pages	March 17, 2025
MI Lecture Note Vol.100	Yutaka Jitsumatsu Masayoshi Ohashi Akio Hasegawa Katsutoshi Shinohara Shintaro Mori	IMI Workshop of the Joint Usage Research Projects Mathematics for Innovation in Information and Communication Technology 274pages	March 19, 2025
MI Lecture Note Vol.101	Makoto Ohsaki Yoshiki Jikumaru	IMI Workshop of the Joint Usage Research Projects Evolving Design and Discrete Differential Geometry:towards Mathematics Aided Geometric Design 528pages	October 1st, 2025
MI Lecture Note Vol.102	Keunsu Kim	Young Researchers and Students-Workshop (I) Topological Data Analysis and Industrial Mathematics 198pages	December 22, 2025

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