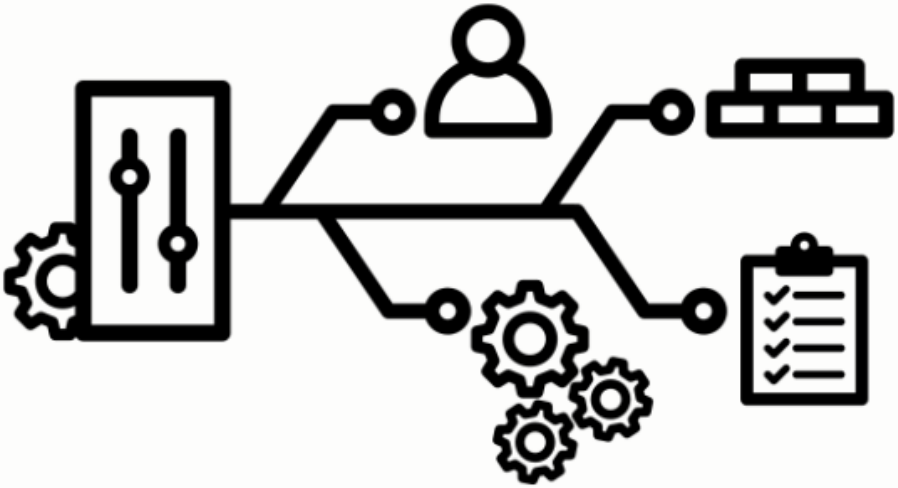
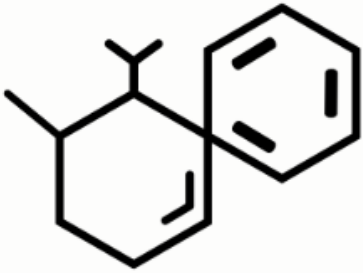


School on Machine Learning for Molecules and Materials Research

June 9, 2025 - June 13, 2025
University of Zadar, Croatia

Book of Abstracts



Contents

General

Organizers

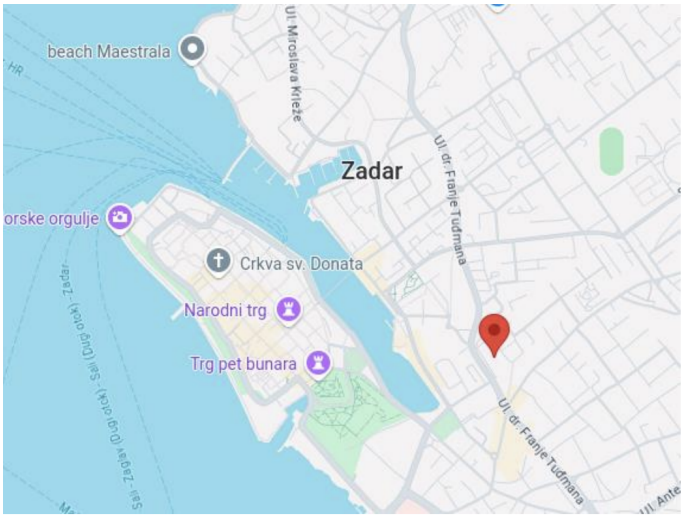
Ivor Lončarić, Ruđer Bošković Institute, Croatia
Kevin Rossi, TU Delft, Netherlands
Federico Grasselli, University of Modena and Reggio Emilia, Italy
Katarina Batalović, Vinča Institute, University of Belgrade, Serbia
Juraj Ovčar, SISSA, Italy / Ruđer Bošković Institute, Croatia

The DAEMON COST Action CA22154 acts as a co-organizer of the event. COST (European Cooperation in Science and Technology) is a funding agency for research and innovation networks. Our Actions help connect research initiatives across Europe and enable scientists to grow their ideas by sharing them with their peers. This boosts their research, career and innovation.

Contents

Venue

- Location: University of Zadar, New Campus
- Address: Ul. dr. Franje Tuđmana 24i, 23000, Zadar, Croatia
- https://maps.app.goo.gl/ghrk4jbUWV7TUb7F8



Poster sessions

There will be two poster sessions, held on Tuesday and Wednesday, 17:15-19:15.
The recommended poster size is A0 portrait.

Meals

Coffee and snacks will be provided to the participants in front of the lecture room.
Lunch will be served on Tuesday, Wednesday, and Thursday in the student restaurant Diadora.
Light finger food and beverages will be served during the poster session.
The social dinner will be held on Thursday evening in the restaurant Barbakan.

Internet Access

An eduroam account is required to access the internet.

Software Requirements for Tutorials

Tutorials can be followed using the Jupyter notebooks hosted at https://jupyter.srce.hr or by self-installation.

Code of Conduct

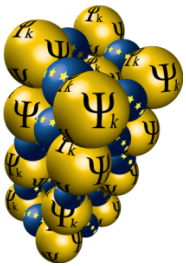
We strive for making every attendee feel welcome and respected. Do not hesitate to contact any of the organizers if you are the witness or the victim of any discrimination or harassment. Step up and speak out to stop any kind of inappropriate behaviour you witness. Bystander intervention creates safer communities and prevents harmful escalation.

Other

The Emergency number for Croatia is 112.

Sponsors

We acknowledge the generous support of CECAM, MaX CoE, Psi-k, University of Zadar, Croatian Science Foundation, SRCE and Ruđer Bošković Institute.



Programme

		09.06.2025.	10.06.2025.	11.06.2025.	12.06.2025.	13.06.2025.
Time		Monday	Tuesday	Wednesday	Thursday	Friday
09:00	09:15		Ilyes	Martin	Johannes	Robert
09:15	09:30		Batatia	Uhrin	Dietschreit	Pinsler
09:30	09:45					
09:45	10:00		Ilyes	Martin	Johannes	Robert
10:00	10:15		Batatia	Uhrin	Dietschreit	Pinsler
10:15	10:30					
10:30	10:45					
10:45	11:00		coffee	coffee	coffee	coffee
11:00	11:15					
11:15	11:30		Jonathan	Panel 1-	Lucas	Andres M
11:30	11:45		Schmidt	future in	Foppa	Bran
11:45	12:00			ML4MD		
12:00	12:15		Jonathan	Panel 2-	Lucas	Andres M
12:15	12:30		Schmidt	future in	Foppa	Bran
12:30	12:45			ML4MD		
12:45	13:00					Closing
13:00	13:15	Registration				
13:15	13:30		lunch	lunch	lunch	
13:30	13:45	Opening				
13:45	14:00	DAEMON				
14:00	14:15	SRCE	Radova	MaX	König	
14:15	14:30	Martin	Corradini	de Gironcoli	Loveday	
14:30	14:45	Belavić	Worakul	Keenan	Pérez De Alba	
14:45	15:00	Nicola	Tristan	Milica	Trezza	
15:00	15:15	Molinari	Bereau	Todorovic	Ramos	
15:15	15:30				Das	
15:30	15:45					
15:45	16:00	coffee	coffee	coffee	coffee	
16:00	16:15					
16:15	16:30	Nicola	Tristan Bereau	Milica	KalphaTech	
16:30	16:45	Molinari	Luis Walter	Todorovic	Rimac Tech	
16:45	17:00					
17:00	17:15					
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17:30	17:45					
17:45	18:00					
18:00	18:15					
18:15	18:30		Poster session	Poster session	Social Dinner	
18:30	-	City tour	1 (17.15-19.15)	2 (17.15-19.15)	(18-21)	

Monday

13:00 - 13:30	Registration
13:30 - 13:45	**Ivor Lončarić (Conference chair)** Opening Remarks
13:45 - 14:00	**Kevin Rossi (DAEMON COST Action chair)** DAEMON COST: a European network on Machine Learning for Materials Science
14:00 - 14:15	**University of Zagreb, University Computing Centre** SRCE Role in Supporting Research through Advanced Computing
14:15 - 14:45	**Martin Belavić** Set up of computers for tutorials
14:45 - 15:30	**Nicola Molinari** Intro Lecture: Modeling Electrolytes, theory and practice
15:30 - 16:15	Coffe Break
16:15 - 17:00	**Nicola Molinari** Tutorial Lecture: Modeling Electrolytes, theory and practice
17:30 - 18:30	**City Tour**

DAEMON COST: a European network on Machine Learning for Materials Science

Kevin Rossi[1]

[1] *Technical University of Delft, Delft, Netherlands*

DAEMON COST [1,2] is a pan-European network consisting of 200+ members from 40+ EU countries, which focuses on capacity-building and research-coordination efforts, with the end goal of popularizing and democratizing emergent approaches, such as generative AI and automated labs, to accelerate materials discovery, design, and commercialization.
In this presentation I will discuss ongoing efforts and activities of the network towards this goal. Next, I will focus on the challenges and opportunities, which characterize materials acceleration in the specific context of a truly horizontal, inclusive, and pan-European network, together with the top-down and bottom-up level policies we aim to lobby for.

[1] https://www.cost.eu/actions/CA22154/

[2] https://cost-daemon.eu/

SRCE Role in Supporting Research through Advanced Computing

Martin Belavić[1]

[1] *University Computing Center, University of Zagreb, Croatia*

SRCE is a central infrastructure institution that plans, develops, and improves e-infrastructure and digital services for the needs of the academic and scientific community in Croatia and provides support in their usage. Advanced computing has become an essential tool across numerous scientific disciplines, including machine learning, artificial intelligence, bioinformatics, computational chemistry, climate modeling, and engineering. By offering cutting-edge computing infrastructure, advanced computing enables researchers to tackle complex challenges that demand substantial computational resources—such as high-performance processors, accelerators, large memory capacities, shared storage, and specialized scientific applications and environments. SRCE will provide participants of the "School on Machine Learning for Molecules and Materials Research" access to Jupyter environment with NVIDIA Multi-Instance GPU (MIG) technology. Each environment will offer between 2 to 8 virtual CPUs and 16 to 24 GB of RAM, ensuring a robust platform for hands-on learning and research.

Modeling Electrolytes, theory and practice

Nicola Molinari[1,2]

[1] *Robert Bosch , Boston, USA*
[2] *Harvard University, Boston, USA*

Electrolytes control efficiency, anode/cathode stability, battery recharge time as well as safety, thus their optimization is crucial for the design of next-generation energy storage device. Here we focus on ionic liquid-based electrolytes thanks to their superior chemical stability compared to standard organic solvents, however, poor and anomalous transport properties are hindering their applicability.

In this talk we will journey through various simulation techniques to shine light on different aspects of such materials. Ultimately, classical energy models struggle to provide the level of accuracy needed to reliably predict and investigate these systems. Thus, we will conclude by exploring the applicability to such systems of state of the art equivariant graph neural networks. Ionic liquid-based electrolytes provide a unique challenge due to their strong ionic interactions and viscous liquid nature. Additionally, substantially diverse inter-atomic environments are often present as a function of lithium-salt doping, raising the interesting question of model transferability.

Tuesday

9:00 - 9:45	**Ilyes Batatia** Intro Lecture: A Dive into MACE Foundation Models for Atomistic Chemistry
9:45 - 10:30	**Ilyes Batatia** Tutorial Lecture: Introduction to MACE training, fine-tuning and active learning.
10:30 - 11:15	Coffee Break
11:15 - 12:00	**Jonathan Schmidt** Intro Lecture: Accelerating Material Science with High-Throughput Searches
12:00 - 12:45	**Jonathan Schmidt** Tutorial Lecture: Accelerating Material Science with High-Throughput Searches
12:20 - 14:00	Lunch Break
14:00 - 14:15	**Mariia Radova** Contributed talk: Fine-tuning foundation models of materials interatomic potentials with frozen transfer learning
14:15 - 14:30	**Andrea Corradini** Contributed talk: Scalable machine learning approach to light induced order disorder phase transitions with ab initio accuracy
14:30 - 14:45	**Thanapat Worakul** Contributed Talk: Exploring Chemical Space for Singlet Fission Materials with Generative Design
14:45 - 15:30	**Tristan Bereau** Intro Lecture: Transferable coarse-grained models accelerate chemical-space exploration
15:30 - 16:15	Coffee Break
16:15 - 17:00	**Tristan Bereau and Luis Walter** Tutorial Lecture: Transferable coarse-grained models accelerate chemical-space exploration
17:15 - 19:15	Poster session

A Dive into MACE Foundation Models for Atomistic Chemistry

Ilyes Batatia[1]

[1] *University of Cambridge, United Kingdom*

In this lecture, we'll start by understanding why traditional electronic-structure methods face limitations and how machine learning force fields offer powerful, efficient alternatives for atomistic simulations. I'll guide you through the key ideas behind the MACE architecture, highlighting how many-body equivariant message-passing networks and tensor decomposition effectively capture local atomic environments. We'll then discuss a transformative shift in the field—from developing system-specific force fields toward creating versatile foundation models. You'll see how models like MACE-MP-0, along with newer versions like MACE-MPA-0 and MACE-OMAT-0, achieve remarkable generalization. Although these models are trained only on small inorganic crystals, they successfully simulate diverse systems, including crystals, liquids, molecules, surfaces, and even complex interfaces. Finally, we'll explore practical strategies for fine-tuning these foundation models. I'll demonstrate how a multi-head fine-tuning approach helps reach quantum-level accuracy while maintaining the robustness of the underlying model, providing clear examples to illustrate this powerful technique.

Introduction to MACE training, fine-tuning and active learning.

Ilyes Batatia[1]

[1] *University of Cambridge, United Kingdom*

In this tutorial, we will introduce you to the basics of MACE training and evaluation. We cover the construction of a dataset, the basic hyperparameters of a MACE model, and how to train and evaluate a model. Then we will show you how to use MACE for active learning and fine-tuning.

Accelerating Material Science with High-Throughput Searches

Jonathan Schmidt [1]

[1] *ETH Zurich, Switzerland*

Advances in computational power, first-principle codes, automation frameworks, materials databases, and machine learning have revolutionized materials research by enabling the rapid screening of vast chemical spaces. We can now survey billions of candidate compounds where we previously had to limit ourselves to thousands.

In the intro lecture session, we will cover the key principles of high-throughput materials searches — using inorganic crystal structures as examples — including selecting a search space, balancing accuracy against throughput, and automation. We will also address practical issues such as securing computational resources and dataset licensing.

In the tutorial session, we will try to discover a novel garnet substrate for Yttrium Iron Garnet spintronics applications. We will build a pipeline using the OPTIMADE API standard for accessing crystal-structure repositories, coupled with the Atomate2 workflow management and universal machine learning models.

Fine-tuning foundation models of materials interatomic potentials with frozen transfer learning

Mariia Radova[1]1

[1] *University of Warwick, United Kingdom*

Machine-learned interatomic potentials are revolutionising atomistic materials simulations by providing accurate and scalable predictions within the scope covered by the training data. However, generation of an accurate and robust training data set remains a challenge, often requiring thousands of first-principles calculations to achieve high accuracy. Foundation models have started to emerge with the ambition to create universally applicable potentials across a wide range of materials. While foundation models can be robust and transferable, they do not yet achieve the accuracy required to predict reaction barriers, phase transitions, and material stability. This work demonstrates that foundation model potentials can reach chemical accuracy when fine-tuned using transfer learning with partially frozen weights and biases. For two challenging datasets on reactive chemistry at surfaces and stability and elastic properties of tertiary alloys, we show that frozen transfer learning with 10-20% of the data (hundreds of datapoints) achieves similar accuracies to models trained from scratch (on thousands of datapoints). Moreover, we show that an equally accurate, but significantly more efficient surrogate model can be built using the transfer learned potential as the ground truth. In combination, we present a simulation workflow for machine learning potentials that improves data efficiency and computational efficiency.

Scalable machine learning approach to light induced order disorder phase transitions with ab initio accuracy

Andrea Corradini, [1] Giovanni Marini, Matteo Calandra

[1] *University of Trento, Italy*

While machine learning excels in simulating material thermal properties, its application to order-disorder non-thermal phase transitions induced by visible light has been limited by challenges in accurately describing potential energy surfaces, forces and vibrational properties in the presence of a photoexcited electron-hole plasma. Here, we present a novel approach that combines constrained density functional theory with machine learning, yielding highly reliable interatomic potentials capable of capturing electron-hole plasma effects on structural properties. Applied to photoexcited silicon, our potential accurately reproduces the phonon dispersion of the crystal phase and allows for molecular dynamics simulations of tens of thousands of atoms. We show that, at low enough temperatures, the non-thermal melting transition is driven by a soft phonon and the formation of a double-well potential, at odds with thermal melting being strictly first order. Our method paves the way to large-scale, long-time simulations of light-induced order-disorder phase transitions with ab initio accuracy.

Exploring chemical space for singlet fission materials with generative design

Thanapat Worakul [1], Rubén Laplaza, J. Terence Blaskovits, Clémence Corminboeuf

[1] *EPFL, Switzerland*
,

We recently introduced the FORMED repository, comprising 116,687 synthesizable molecules, which was leveraged for fragment-based high-throughput virtual screening (HTVS) and genetic algorithm (GA) searches to identify singlet fission (SF) molecular candidates. These approaches successfully identified both prototypical SF chromophores (e.g., acenes, boron-dipyrromethane (BODIPY)) and previously unrecognized candidates (e.g., heteroatom-rich mesoionic chromophores) that satisfy stringent SF energetic criteria. However, the reliance on predefined molecular fragments and heuristic structure generation rules constrains the scope of chemical space exploration, thereby limiting the discovery of entirely novel molecular scaffolds.

To overcome these limitations, here, we employ a generative learning framework that integrates REINVENT, a molecular generative model, with Chemprop, a property prediction model, driven by reinforcement learning. This approach enables the generative model to rediscover a diverse range of previously reported SF chromophore classes while also proposing previously unreported SF scaffold not found in the training data. This work highlights the potential of generative design's ability to not only discover diverse potential molecules but also uncover new candidates for tailored material applications.

References

[1]T. Worakul, R. Laplaza, J. Blaskovits, C. Corminboeuf, Generative Design of Singlet Fission Materials by Revisiting the Use of a Fragment-oriented Database, 2025

Transferable coarse-grained models accelerate chemical-space exploration

Tristan Bereau , Luis Walter[1]

[1] *Heidelberg University, Germany*

Advanced statistical methods are rapidly impacting many scientific fields, offering new perspectives on long-standing problems. In materials science, data-driven methods are already bearing fruit in various disciplines, such as hard condensed matter or inorganic chemistry, while comparatively little has happened in soft matter. I will describe how we use multiscale simulations to leverage data-driven methods in soft matter. We aim at establishing structure-property relationships for complex thermodynamic processes across the chemical space of small molecules. Akin to screening experiments, we devise a high-throughput coarse-grained simulation framework. Coarse-graining is an appealing screening strategy for two main reasons: it significantly reduces the size of chemical space and it can suggest a low-dimensional representation of the structure-property relationship. I will describe how we accelerate molecular discovery by blending representation learning, free-energy calculations, and a Bayesian-optimization framework. We used this framework in the context of a complex biomolecular problem that led to the discovery of in vivo active compounds. Finally, I will discuss how exploiting the hierarchical nature of coarse-grained models can further accelerate the exploration of chemical space.

Wednesday

09:00 - 9:45	**Martin Uhrin** Intro Lecture: Physics-Informed Machine Learning of Response Properties for Atomic Structure Determination
09:45 - 10:30	**Martin Uhrin** Tutorial Lecture: Physics-Informed Machine Learning of Response Properties for Atomic Structure Determination
10:30 - 11:15	Coffee Break
11:15 - 12:45	**Panel Discussion** Theme: Machine Learning for Molecules and Materials Research Future
12:45 - 14:00	Lunch Break
14:00 - 14:15	**Federico Grasselli** MaX and Lhumos: Building Skills and Tools for High-Performance Computational Materials Science
14:15 - 14:30	**Stefano de Gironcoli** Contributed Talk: Toward General-Purpose Machine Learning Interatomic Potentials
14:30 - 14:45	**Luke Keenan** Contributed Talk: Machine Learning accelerators for quantum transport
14:45 - 15:30	**Milica Todorovic** Intro Lecture: Bayesian optimization of materials and molecular properties
15:30 - 16:15	Coffee Break
16:15 - 17:00	**Milica Todorovic** Tutorial Lecture: Bayesian optimization of materials and molecular properties
17:15 - 18:30	Poster session

Physics-Informed Machine Learning of Response Properties for Atomic Structure Determination

Martin Uhrin[1]

[1] *Multidisciplinary Institute in Artificial Intelligence, Université Grenoble Alpes, Grenoble, France*

Determining atomic-scale structure from experimental measurements is a longstanding challenge in materials science, especially in systems lacking long-range order or where multiple structural models are consistent with the data. In this lecture and tutorial, we will focus on how machine learning models informed by physical symmetries can be used to predict response properties - such as NMR chemical shifts, Raman spectra, and Born effective charges - that are directly accessible through experiment and highly sensitive to local atomic environments.

A central theme will be the use of equivariant neural networks, which respect the geometric and tensorial nature of physical quantities by construction. These models provide a natural and robust framework for learning complex properties with fewer data and stronger generalization. We will explore two complementary approaches: direct prediction of response tensors, and derivative-based prediction using automatic differentiation through energy models.

Participants will gain hands-on experience with our in-house suite of high-performance, JAX-based Python libraries - tensorial, e3md, and e3response - designed for scalable training and inference across different computing architectures. By the end of the session, attendees will have a working understanding of how to build and deploy these models in structure determination workflows, as well as an appreciation for the underlying physics that make them effective.

MaX and Lhumos: Building Skills and Tools for High-Performance Computational Materials Science

Federico Grasselli[1,2]

[1] *Dept. Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Italy*
[2] *CNR-Nano, Modena, Italy*

MaX (MAterials design at the eXascale) is a European Centre of Excellence focused on advancing computational materials science by leveraging the power of high-performance computing (HPC) within the EuroHPC ecosystem. MaX develops cutting-edge open source community codes for quantum simulations of materials, optimized for current and future exascale architectures.

In this talk, I will introduce the core mission of MaX, providing a special emphasis on MaX's comprehensive strategy to train users of materials science codes as well as a new generation of developers. Furthermore, I will introduce the Lhumos platform (Learning HUb for MOdeling and Simulation), an innovative e-learning resource designed to support training in computational science, particularly within the materials science domain. Lhumos is developed with the support of MaX in collaboration with European initiatives as CECAM and MARVEL, and aims to upskill students, scientists, and industrial users in HPC applications and atomistic simulations, therefore aligning with MaX's broader goal of building a community ready for advanced research in computational materials science.

Toward general-purpose machine learning interatomic potentials

Stefano de Gironcoli[1],

[1] *Scuola Internazionale Superiore di Studi Avanzati (SISSA) - Trieste, Italy*

Machine learning interatomic potentials are transforming atomistic simulations promising to deliver the accuracy of first-principles calculations at a fraction of their cost. It is now established that accurate potentials can be obtained for a specific system if enough accurate data of all the relevant phases are computed and included in the training phase. A number of state-ofthe-art architechtures have been proposed to this end. Challenges remain to develop generalpurpose "foundational" models which can deal accurately and efficiently with systems of arbitrary stoichiometry, interpolating in the chemical space, incorporating long-range electrostatics for metals and insulators as well as van der Waals interactions when necessary, and efficiently leveraging the wealth of, not necessarily mutually consistent, ab-initio calculations available, avoiding as much as possible the need to repeat expensive calculations to improve consistency and chemical/structural coverage. I'll discuss some of these issues and our attempts to address them [1, 2, 3, 4, 5].

References

[1] R. Lot, F. Pellegrini, Y. Shaidu, and E. Küçükbenli , PANNA: Properties from Artificial Neural Network Architectures, Comput. Phys. Commun. 256, 107402 (2020). https://doi.org/10.1016/j.cpc.2

[2] Y. Shaidu, E. Küçükbenli, R. Lot, F. Pellegrini, E. Kaxiras and S. de Gironcoli, A systematic approach to generating accurate neural network potentials: the case of carbon, npj Comput. Mater. 7, 52 (2021). https://doi.org/10.1038/s41524-021-00508-6

[3] F. Pellegrini, R. Lot, Y. Shaidu, and E. Küçükbenli, PANNA 2.0: Efficient neural network interatomic potentials and new architectures, J. Chem. Phys. 159, 084117 (2023). https://doi.org/10.1063/5.0

[4] F. Pellegrini, S. de Gironcoli, and E. Küçükbenli, LATTE: an atomic environment descriptor based on Cartesian tensor contractions, arXiv 2405.08137v1 (2024).

[5] Y. Shaidu, F. Pellegrini, E. Küçükbenli, R. Lot, and S. de Gironcoli, Incorporating long-range electrostatics in neural network potentials via variational charge equilibration from shortsighted ingredients, npj Comput. Mater. 10, 47 (2024). https://doi.org/10.1038/s41524-024-01225-6

Machine Learning accelerators for quantum transport

Luke Keenan[1]

[1] *Trinity College Dublin, Ireland*

The non-equilibrium Green's functions (NEGF) method for quantum transport combined with DFT (NEGF+DFT) is the current state of the art for microscopic quantum transport calculations, and the Smeagol code, developed and maintained by the computational spintronics group at Trinity College Dublin, is at present the world-leading software for this task. Unfortunately, although Smeagol is highly efficient, the computational overheads of a linear-response transport calculation are typically hundred times larger than those of a standard DFT one, and they grow to about a thousand times at finite bias. This limits enormously the size and type of problem that one can tackle. The crux of the matter is that one has to calculate the non-equilibrium electron density, an operation that requires the computation of the junction Green's function over an energy grid. Recently, the group has developed a machine-learning cluster expansion (the Jacobi-Legendre expansion) to compute the charge density of equilibrium DFT calculations. This requires a very limited number training points still achieving extremely high accuracy. Here we propose to extend such formalism to open systems so to bypass completely the construction of the Green's function.

Thus the grand challenge of ML-transport is to establish a ML approach to the NEGF+DFT method enabling a massive speedup. The project has then three main objectives: 1) Develop a cluster expansion method for the non-equilibrium charge density 2) Integrate the cluster expansion into the Smeagol code 3) Demonstrate the efficacy of the method with temperature-dependent quantum transport calculations

This is the first attempt to tackle the problem in a very general way, providing a single solution for the calculation of the non-equilibrium charge density and hence the transport properties. As such, it will be agnostic of the specific device or material and will be employed in a universal way.

Bayesian optimization of materials and molecular properties

Milica Todorović[1]

[1] *University of Turku, Finland*

The arrival of materials science data infrastructures in the past decade has ushered in the era of data-driven materials science based on artificial intelligence (AI) algorithms, which has facilitated breakthroughs in materials optimization and design. Of particular interest are active learning algorithms, where datasets are collected on-the-fly in the search for optimal solutions. We encoded such a probabilistic algorithm into the Bayesian Optimization Structure Search (BOSS) Python tool for materials optimization [1].

BOSS builds N-dimensional surrogate models for materials' energy or property landscapes to infer global optima, allowing to conduct targeted materials engineering. The models are iteratively refined by sequentially sampling density-functional theory (DFT) data points with high information content. This creates compact and informative datasets. We utilized this approach to study molecular surface adsorbates [2], thin film growth [3], solid-solid interfaces [4], molecular conformers [5] and even optimise experimental outcomes [6].

This tutorial will introduce the concepts of active learning and the key choices in Bayesian optimization, before focusing on its implementation in materials simulations and the quality monitoring needed to reach optimal solutions.

References

[1] npj Comput. Mater., 5, 35 (2019)
[2] Beilstein J. Nanotechnol. 11, 1577-1589 (2020), Adv. Func. Mater., 31, 2010853 (2021)
[3] Adv. Sci. 7, 2000992 (2020)
[4] ACS Appl. Mater. Interfaces 14 (10), 12758-12765 (2022)
[5] J. Chem. Theory Comput. 17, 1955 (2020)
[6] J Lofgren ACS Sustain. Chem. Eng. 10, 9469-9479 (2022)

Thursday

09:00 - 09:45	**Johannes Dietschreit** Intro Lecture: Designing Machine Learning Models for Nonadiabatic Dynamics
09:45 - 10:30	**Johannes Dietschreit** Tutorial Lecture: Designing Machine Learning Models for Nonadiabatic Dynamics
10:30 - 11:15	Coffee Break
11:15 - 12:00	**Lucas Foppa** Intro Lecture: Modelling Materials' Properties via the "Materials Genes" Concept: Integrating Theoretical and Experimental Data
12:00 - 12:45	**Lucas Foppa** Tutorial Lecture: Training Subgroup-Discovery and SISSO Models of Materials' Properties*
12:45 - 14:00	Lunch Break
14:00 - 14:15	**Patricia Koning** Contributed Talk: Physics-Based Generative Models: Improved Sampling for Inverse Materials Design
14:15 - 14:30	**Oliver Loveday** Contributed Talk: Automated Frameworks for Reaction Networks in Heterogeneous Catalysis
14:30 - 14:45	**Alberto Perez de Alba** Contributed: Novel Bayesian approaches to predict and design free-energy landscapes
14:45 - 15:00	**Giovanni Trezza** Contributed Talk: Quantifying and mitigating data bias in materials AI: from model robustness to Energy-GNoME
15:00 - 15:15	**Patricia Ramos** Contributed Talk: A Multimodal Deep Learning Framework for Predicting Structure-Property Relationships in Periodic Materials
15:15 - 15:30	**Mandira Das** Contributed Talk: Unraveling the Surface Chemistry of Aerosols: Interpreting XPS spectra using DFT and Machine Learning
15:30 - 16:15	Coffee Break
16:15 - 16:30	**Kalpha Tech** Contributed Talk: Powder X-ray diffraction for materials - solving the analysis bottleneck
16:30 - 16:45	**Rimac Tech** Contributed Talk
18:00 - 21:00	Social Dinner

Designing Machine Learning Models for Nonadiabatic Dynamics

Johannes Dietschreit [1]

[1] *University of Vienna, Austria*

Machine learning (ML) has become an indispensable tool for modeling potential energy surfaces and forces in molecular systems. However, its application to *nonadiabatic dynamics* poses unique challenges, where the interactions between electronic states play a central role. This talk will give an overview of how ML models can be used in this context, with a focus on the critical role of model architecture when predicting quantities like nonadiabatic couplings, quantities that may be highly sensitive to small geometric perturbations. Drawing on concrete examples, I will try to outline strategies for designing architectures that respect the underlying physics.

Modelling Materials' Properties via the "Materials Genes" Concept: Integrating Theoretical and Experimental Data

Lucas Foppa[1]

[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*

The intricate interplay of underlying processes governing certain materials' properties and functions prevents the explicit, atomistic modelling and hinders the efficient design of new materials. In this talk, I will discuss AI approaches that combine theory and experiment to identify the key descriptive parameters ("materials genes") correlated with the materials' performance and reflecting the relevant physical underlying processes that trigger, facilitate, or hinder the materials' behavior. The symbolic-regression sure-independence-screening-and-sparsifying-operator (SISSO) and the subgroup-discovery (SGD) AI methods leverage the typically small high-quality experimental datasets in materials science and identify nontrivial relationships between multiple key descriptive parameters and the performance, thus guiding the design of new, improved materials. The "materials genes" concept will be illustrated for heterogeneous catalysis as an example of a complex materials' function.[1,2,3]

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Training Subgroup-Discovery and SISSO Models of Materials' Properties

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In the tutorial, we will reproduce/modify the analysis discussed in reference [1] by using a jupyter notebook. An executable file for the realkd (java) code will be provided for the subgroup-discovery analysis, which can be run from the Jupyter notebook locally in a laptop. The SISSO analysis for this example will focus on post-processing of provided SISSO output files, since training the models of that publication requires HPC. However, I will also show how to train SISSO models for a simpler example by using the NOMAD AI Toolkitcan be run by using a web browser.

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Physics-Based Generative Models: Improved Sampling for Inverse Materials Design

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Data-driven approaches for inversely designing novel materials with desired properties have become a key aspect in materials discovery. Here, we introduce a framework using physics-based Generative Adversarial Networks for enhanced structure-property sampling via latent space design.

We are interested in sampling structures of two chemical systems that correspond to different physical quantities, like the work function in the electrochemical adsorption of Iodide and Hydroxide on Copper surfaces, and the oxygen chemical potential in the CO to CO2 conversion over the amorphous RuO2 catalyst. To generate physically meaningful structures, we track and evaluate the the structural diversity and convergence of our generator with machine-learning interatomic potentials and quantitative metrics. Our framework enables a high throughput and cost-effective evaluation of structural guesses and their related properties to leverage the full potential of generative models.

Concluding, we are showing on two model systems how to explore a vast chemical space of datasets with sparse areas, particularly structures with high free energies in transition states and diverse amorphous surface structures, thereby advancing the understanding and design of novel materials.

Automated Frameworks for Reaction Networks in Heterogeneous Catalysis

Oliver Loveday [1,2], S. Morandi[1,2], T. Renningholtz[1], S. Pablo-García[3,4,5],R. A. VargasHernández[6], R. Rohit Seemakurthi[1], P. Sanz[1,2],R. García-Muelas[1],A. Aspuru-Guzik[3,4,5],N. López[1,*]

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[4] *Department of Computer Science, University of Toronto, Sandford Fleming Building, 40 St. George Street, ON M5S 2E4, Toronto, Canada;*
[5] *Vector Institute for Artificial Intelligence, 661 University Ave. Suite 710, ON M5G 1M1, Toronto, Canada;*
[6] *6 Department of Chemistry Chemical Biology, MacMaster University 1280 Main Street West, L8S 4L8, Hamilton, Canada;*
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The study of reaction mechanisms in heterogeneous catalysis has traditionally relied on chemical intuition for proposing paths and density functional theory (DFT) simulations to evaluate them. While this approach has been key in explaining experimental reactivity trends, it overlooks alternative paths that could likely have a key role in the overall process, and finds its limits when applied to complex mechanisms. To overcome this limitation and target a more realistic description of catalytic systems, new strategies involving automation and machine learning (ML) tools are key to obtain a more complete construction and evaluation of chemical reaction networks (CRNs).1 Herein we present a modular framework capable of (i) automatically identify and generate all the potentially involved species and reactions, (ii) evaluate the groundstate and transition state energies for the species via state-of-the-art machine learning interatomic potentials (MLIPs), mainly powered by a built-in graph neural network GAME-Net-UQ, able to provide robust predictions comparable to DFT and, (iii) the inclusion of a mean-field microkinetic model (MKM) to further expand the analysis. To showcase its capabilities, several case studies are investigated and features such as catalytic activity, selectivity and breaking the limits of traditional methodologies by achieving the study of previously untreatable complex CRNs, paving the way towards the exploration and analysis these kinds of catalytic processes. [2]

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[2] S. Morandi, O. Loveday, et al., 10.26434/chemrxiv-2024-bfv3d (2024) Acknowledgments This work was supported by the Joan Oró Predoctoral Programme of the Secretariat of Universities and Research of the Department of Research and Universities of the Generalitat de Catalunya, and the European Social Fund Plus. Reference: 2023 FI-1 00769d; NCCR Catalysis (grant number 180544); and the BSC-RES for generously providing computational resources.

Novel Bayesian approaches to predict and design free-energy landscapes

Alberto Pérez De Alba Ortíz [1]

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To dissect and control atomistic processes, it is essential to map their free-energy landscape. This landscape reveals metastable states and interconnecting paths—projected onto key atomistic descriptors—which are crucial to understand chemical, conformational or phase transitions. Since most interesting processes are rare events within affordable simulations, multiple enhanced sampling methods have been introduced. Many of these methods exert biasing potentials to drive the system into unsampled regions. The average biasing force can be used to numerically integrate an approximation of the free-energy landscape. However, determining where to set the biasing potentials can be daunting for complex systems involving many descriptors. To tackle this, we employ Bayesian quadrature as a method to estimate the value of an integral, i.e., the free energy, based on iteratively selecting the most informative gradient samples, i.e., forces, based on a noise-tolerant probabilistic model. This approach can either explore the landscape by reducing the overall uncertainty or exploit it by searching for minima or maxima. We demonstrate the robustness of this approach across novel applications to relevant molecules and materials, including predictions of biopolymer rigidity, metal phase transitions, nanoplastic-induced protein dissociation, etc.

Quantifying and mitigating data bias in materials AI: from model robustness to Energy-GNoME

Giovanni Trezza [1], Paolo De Angelis, Giulio Barletta, Pietro Asinari, Eliodoro Chiavazzo

[1] *Politecnico di Torino, Italy*

Exploiting high-quality data is crucial for reliable Artificial Intelligence (AI)-driven materials discovery. However, biases arising from non-random, intuition-driven sample selection during database creation can negatively affect predictive accuracy when models trained on specialized datasets are applied to materials of different genesis. Such bias may persist despite using large, reputable databases, ultimately hindering the effectiveness of AI models.

To overcome this issue, we introduce a methodology designed to detect and quantify data bias, thus enhancing model reliability. Our approach employs a fully supervised strategy that identifies and excludes out-of-domain materials for which model predictions may be unreliable. Validated through case-studies on superconducting and thermoelectric materials, our pipeline demonstrates the ability to mitigate bias effects, showcasing flexibility and potential ease of integration into various AI architectures, including modern equivariant graph-based neural networks.

We applied this methodology to screen the recently released GNoME database, encompassing over 380,000 AI-generated structures, to identify those exhibiting promising values for several key properties, including thermoelectric figure of merit, band gap, and cathode voltage. Additionally, we provided an online platform that enables rapid exploration of these predicted properties and offers insights into their potential reliability (https://paolodeangelis.github.io/Energy-GNoME/).

A Multimodal Deep Learning Framework for Predicting Structure-Property Relationships in Periodic Materials

Patrícia Ramos[1,2], José Oliveira[1,3]

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[2] *Polytechnic of Porto, Portugal;*
[3] *University of Porto, Portugal*

Multimodal Machine Learning (MLL) is an advanced technique that is gaining significant traction across various domains, including robotics, computer vision, and natural language processing. By integrating multiple data sources, such as text, images, audio, and video, MLL enhances model performance while mitigating inconsistencies inherent in single-modality data. One of its most powerful capabilities is cross-modal knowledge transfer, where insights derived from one modality inform and refine another, leading to improved generalization and adaptability. Compared to unimodal models, which rely on a single data type, multimodal approaches often yield more robust and accurate predictions [1].

Despite its widespread success in other fields, multimodal learning remains largely underexplored in materials science. However, leveraging multimodal approaches in this domain has the potential to significantly enhance predictive accuracy in materials discovery [2-4]. This study introduces a multimodal deep learning framework designed to predict the properties of periodic materials by integrating diverse data modalities. The proposed methodology incorporates multiple data representations, including chemical composition (text-based), crystal structure (graph-based), spectroscopic data (image-based), and material properties (tabular-based). By fusing these modalities, the model aims to improve the accuracy and reliability of structure-property predictions, directly contributing to materials generation and experimental validation.

To effectively integrate these diverse data sources, we employ an early fusion strategy [5], where feature representations from different modalities are merged into a unified vector before training. This approach enables the model to capture intricate cross-modal interactions, enhancing its ability to learn complex structure-property relationships. To achieve this, we utilize specialized deep learning architectures tailored to each data type within the materials domain. Chemical composition data is processed using Roost [6], which captures element-wise relationships and stoichiometric patterns. Crystal structures are modeled with CGCNN [7], a graph neural network designed to encode atomic connectivity and structural interactions. Spectroscopic data, particularly X-ray diffraction (XRD) patterns, are analyzed using a Vision Transformer to extract key diffraction features. Additionally, key material properties represented as tabular data are processed using FT-Transformer [8], a Transformer-based model optimized for capturing intricate feature interactions and improving predictive performance.

To rigorously evaluate the proposed framework, we assess prediction accuracy using Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) metrics on a publicly available dataset. This evaluation provides a comprehensive measure of model performance across different data modalities, ensuring robustness and reliability in materials property prediction.

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Unraveling the Surface Chemistry of Aerosols: Interpreting XPS spectra using DFT and Machine Learning

Mandira Das [1]

[1] *University of Turku, Finland*

Aerosols, air-suspended nano to micro sized particles have significant impact on the climate, weather, health and ecology. The size and compositions of aerosol particles affect their interactions with atmospheric compounds. Sodium Chloride (NaCl) is the most abundant aerosol particle. Surface-sensitive Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) reveals that NaCl aerosol particles undergo structural changes depending upon the varying humidity of the atmosphere [1]. However, identifying the surface atomic arrangement behind the interaction of NaCl aerosol with atmosphere under humid conditions remains challenging.

To overcome this challenge, we investigate the surface structure and interaction of aerosols under humid conditions using density functional theory (DFT) and machine learning (ML).

We applied Bayesian Optimization (BO) in conjunction with DFT to model the adsorption geometry of the atmospheric water on the NaCl aerosol surface. We used Bayesian Optimization Structure Search (BOSS) [2] code that can sample different configurations of atmospheric water on the aerosol surfaces to learn the adsorption energy landscapes. After optimizing the adsorption geometry, we employed the self-consistent field (SCF) [3] approach to calculate the core electron binding energy of the Na 1 s electron of the NaCl aerosol particles. The changes in XPS spectra under humid conditions can be explained by comparing binding energy of Na 1s before and after adsorption of atmospheric water. This study uses ML-driven DFT to unveil atomic scale interactions of the aerosols with atmospheric water, explaining APXPS data and serves as a roadmap to explore interactions of more complex atmospheric compounds with aerosols.

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Powder X-ray diffraction for materials - solving the analysis bottleneck

Stipe Lukin [1]

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Laboratory and industrial automation are driving significant advancements in materials synthesis and discovery, often operating 24/7 with the aid of autonomous robots. 1 This rapid production capability has shifted the bottleneck in materials science from synthesis to efficient characterization. 2 Powder X-ray diffraction (PXRD) remains a crucial technique for solid materials analysis across various industries, including pharmaceutical, chemical, and cement. 3 Beyond qualitative and quantitative analysis, PXRD is essential for determining crystal structure and texture (particle size and strain). This presentation will highlight how in KalphaTech we use ML to move the process of structure characterization from typically days to less than 30 minutes.

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Friday

09:00 - 09:45	**Robert Pinsler** Intro Lecture: Generative models for molecules and materials
09:45 - 10:30	**Robert Pinsler** Tutorial Lecture: Generative models for molecules and materials
10:30 - 11:15	Coffee Break
11:15 - 12:00	**Andres M. Bran** Intro Lecture: Towards Autonomous Reasoning Agents in Chemistry
12:00 - 12:45	**Andres M. Bran** Tutorial Lecture: Towards Autonomous Reasoning Agents in Chemistry
12:45 - 13:00	**Closing Remarks** Closing

Generative models for molecules and materials

Robert Pinsler [1]

[1] *Microsoft Research, United Kingdom*

Finding chemical compounds with desirable properties is a challenging task with important applications in de novo drug design and materials discovery. While an exhaustive search of the entire space of possible structures is hopeless, generative models have the potential to directly propose new compounds with target properties. In the first part of this talk, I will provide an overview of different generative modeling approaches for molecules and materials. In the second part, I will take a closer look at MatterGen, a state-of-the-art diffusion model for generating stable, diverse inorganic materials across the periodic table that can be fine-tuned to steer the generation towards a broad range of property constraints.

Towards Autonomous Reasoning Agents in Chemistry

Andres M. Bran [1]

[1] *EPFL , Switzerland*

The integration of artificial intelligence and chemistry has rapidly evolved in recent years [1], partially driven by accelerated advances in Large Language Models (LLMs) and their increasing abilities to understand and reason about chemical concepts. This evolution is mirrored and led by our research, initially with the development of ChemCrow [2], an LLM-based agent capable of using specialized chemical tools to bridge the gap between computational and experimental chemistry. This enabled autonomous planning and execution of complex tasks including organic synthesis and collaborative materials design. Further experiments showed that LLMs could serve as powerful chemical reasoning engines, capable of understanding and applying chemical principles to under-specified and abstract tasks, mimetizing thinking of expert chemists. Leveraging this we could build systems that can reason through vast chemical spaces, to tackle strategic synthesis planning and mechanism elucidation, all guided by natural language [3]. In this talk I will illustrate the field's progression through the lens of language and reasoning, a paradigm shift that opens new and exciting possibilities for scientific discovery. As the synergy between AI and chemistry evolves, new ways of doing chemistry appear, along with new approaches to solving long-standing problems in chemistry.

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Posters

Poster Session

Anastasiia Kholtobina
Exploring mechanical properties of molecular crystals with universal machine learning interatomic potentials

Apolinario Tan
Convergence of body-orders in linear atomic cluster expansions

Barbara Pem
Contribution of non-polar amino acids to the binding of cationic peptides to lipid membranes

Bernhard Kretz
Machine-learned excited state potential energy surfaces of nano-porous graphene

Branislav Milovanović
Exciton dynamics in molecular assemblies of perylene-dimiide

Bruno Mladineo
A Machine Learning Approach to Study of Thermosalient Molecular Crystals

Cyprien Bone
Finetuning Large Language Models for Materials Chemistry

Daniel López Díaz
Simulating Electronic Excitations during Photoisomerization of Photoswitch–Quantum Dot Systems

Davide Alimonti
Melting And Freezing Of Aluminium Nanoparticles With A Machine-learnt Potential

Francesca Menescardi
A novel neural network potential to determine the phase boundaries of CaO through non-equilibrium free-energy calculations

Francesco Cosimo Castellucci
A Machine Learning approach targeting the screened potential of 2D materials in the GW approximation

Gordana Marković
Machine Learning-Based Prediction of Biocompatible Titanium Alloys with Low Elastic Modulus

Haseena Sheik
Study of photorelaxation pathways in 7H and 9H tautomers of 2,6-diaminopurine

Ivana Nikšić-Franjić
Computational Design of Chiral Catalysts

Jorge Laranjeira
Helium Compression Chamber: a viable alternative to in silico study of reaction mechanisms under pressure

Khuram Shahzad
Quantum benchmarking of molecular ground-state energy estimation

Lisa Schröder
Accelerating Mechanism Elucidation of Stereoselective Reactions through Machine Learning

Liudmyla Klochko
Transfer Learning for Deep Learning-based Prediction of Lattice Thermal Conductivity

Luca Grisanti
Atomistic modeling of molecular aggregates to understand their properties

Luka Benić
Exploring CDW transitions in monolayer $NbSe_2$ using machine learning techniques

Luoxuan Peng
Atomistic simulation of Ge/SiGe interfaces for quantum technology devices

Maria Incoronata Sciancalepore
Molecular Dynamics Simulations for Sustainability

Matteo Barduzzi
Ab initio DFT calculations of thermoelectric properties of InAs-InAsSb nanowire heterostructures, speeded up by Machine Learning

Mattia Ragni
Data efficient physics informed graph neural network for predicting NMR shielding tensors

Milica Ritopecki
Machine Learning and DFT Insights into the Reducibility and Structural Complexity of InO

Mina Taleblou
Elemental representation in LATTE

Nan Cao
Machine learning for predicting the magnetic properties of carbon-based nanostructures

Nataša Knežević
Application of Machine Learning in the synthesis and characterization of ecofriendly materials for water pollutant removal

Nian Wu
Machine learning interatomic potentials for dynamic simulations of Cu-water-salt interface systems

Pol Sanz
Efficient Strategies for Constructing Robust Machine Learning Potentials

Radovan Matula
Universal Machine Learning Potentials for Molecular Crystals

Rafał Stottko
RGBChem: Image-like Representation of Chemical Compounds for Properties Prediction

Ruoyan Jin
Data-efficient machine learning interatomic potential for studying radiation effects in Ge

Saara Sippola
Active Learning Structure Search Study of 17-Beta-Estradiol Adsorption on Graphene

Saffron Luxford
Data Generation and Physics-Informed Strategies for Machine-Learned Force Fields in Molecular Dynamics

Santiago Mosca
Automation of the Recognition of Crystalline Structures in Molecular Dynamics Simulations by Machine Learning

Sofia Zinzani
Bridging the modeling gap in heterogeneous catalysis via machine learning

Tomasz Galica
Mapping materials space: graph-based representation using ForceAtlas2 and MEGNet