

Useful Information

The **Talks** will take place in the **Dirac amphitheater** , located on the ground floor of the Dirac building, Doua Site.

The coffee breaks and the poster sessions will take place in the IP2I library, located on the **4th floor** of the same **Dirac** building.

Wi-Fi will be available using eduroam.

The **lunch** will be held on the first floor of the '**Domus**' building. See the map on the first page.

How to get to the Doua site?

From the Part-Dieu, you can take tram line T1 towards IUT Feyssine or T4 towards La Doua Gaston Berger. Get off at the Université Lyon 1 stop.

Organizing committee

Pavel AFANASIEV (IRCE)	Abdulrahman ALLOUCHE (iLM)	Guillaume BAULIEU (IP2I)
Colin BOUSIGE (LMI)	Olivier COCHET-ESCARTIN (iLM)	Eric EHRET (IRCE)
Guillaume HOFFMANN (ISA)	Pierre MIGNON (iLM)	Damien MONTARNAL (CP2M)
Olivier PIERRE-LOUIS (iLM)	Olivier STEZOWSKI (IP2I)	Gael TRAN (ICBMS)

Timetable

CT: Contributed Talk, **IS**: Invited Speaker.

Monday, 2 of June

13:30–14:00	Registration		
14:00–14:05	Welcome remarks		
14:05–14:15	IS	Christophe Morell Chargé de mission, Sciences Formelles et appliquées à Lyon 1	Inauguration by the representative of the Lyon 1 Research Presidency
Chairman	Colin Bousige		
14:15–15:45	IS	Jean-Luc Parouty Grenoble, France	Bases, concepts, enjeux et limites de l'IA, dans la Science, pour soi et dans la société.
15:45–16:15	Coffee		
16:15–17:15	IS	Teodoro Laino IBM-Zurich, Switzerland	Fueling the Digital Chemistry Revolution with Language and Multimodal Foundation Models

Tuesday, 3 of June

Chairman	Pierre Mignon		
9:00-10:00	IS	Jörg Behler Bochum, Germany	Four Generations of Neural Network Potentials
10:00-10:30	IS	Tristan Albaret iLM, Villeurbanne, France	TRIP effect in Zirconia: atomistic simulations using neural network interatomic potentials
10:30-11:00	Coffee & Posters		
Chairman	Guillaume Hoffmann		
11:00-11:20	CT	Colin Bousige LMI, Villeurbanne, France	High-dimensional neural network potential for borophene on metallic surfaces
10:20-11:40	CT	Chloé Sanz iLM, VilleurbanneFrance	A Neural Network Atomistic Potential for Pyrophyllite Clay Simulations
11:40-12:00	CT	Florian E.C. Blanc ISA, Villeurbanne, France	Mechanism of Ag ⁺ -induced folding of a bacterial peptide from molecular dynamics simulations and deep dimensionality reduction
12:00-12:20	CT	Steve Jatiere iLM, Villeurbanne, France	Identifying conformational states of TRP-Cage using dimensionality reduction and clustering methods
12:30-14:00	Lunch		
Chairman	Damien Montarnal		
14:00-15:00	IS	Beatriz MOYA Arts et Métiers Institute of Technologie, Paris, France	Physics-informed and augmented learning in fluids and solid mechanics
15:00-15:30	IS	Victor Sabanza Gil Lausanne, Switzerland	Bayesian Optimization for chemical research
15:30-16:00	CT	Sofiane Ferchichi CP2M, Villeurbanne, France	Process Analytical Technology (PAT) at polyolefin recycling service: real-time monitoring using in-situ spectroscopy and chemometrics
16:00-16:30	Coffee & Poster		
Chairman	Olivier Pierre-Louis		
16:30-17:00	IS	Li Fu Ecole Centrale, Lyon, France	Metainterfaces with specified friction laws : new designs from numerical optimization
17:00-17:30	IS	Roland Denis ICJ, Villeurbanne,France	Approximation of mean curvature flows by an interpretable data- driven neural network
17:30-18:00	CT	Matthias Hillenkamp, iLM, Villeurbanne, France	How unsupervised machine learning can provide benchmark input for nanoalloy design

Wednesday, 4 of June

Chairman	Pavel Afanasiev		
9:00 – 10:00	IS	David Rousseau Angers, France	Deep Scopie: an introduction to machine learning for imaging
10:00–10:20	CT	Olivier Cochet-Escartin iLM, Villeurbanne, France	Small, hand-designed Convolutional Neural Networks for biomedical image analysis
10:20-10:40	CT	Joanne Boulos LIRIS, Villeurbanne, France	Image processing and deep learning for the characterization of polluted soils and their petrophysical properties
10:40–11:10	Coffee & Posters		
Chairman	Olivier Coshet-Escartin		
11:10–12:00	IS	Vincent Motto-Ros iLM, Lyon, France	LIBS hyperspectral imaging with AI: a strong analytical potential
12:00–12:30	CT	Hugo Lilti IRCE, Lyon, France	Convolutional Neural Network trained with Attenuated Total Reflectance for hydroxyl quantification in lignin
12:30–14:00	Lunch		
Chairman	Laetitia Matignon		
14:00–15:00	IS	Aurélien Garivier ENS, Lyon, France	Introduction to Reinforcement learning
15:00–16:00	IS	Aurore Loisy Marseille, France	Reinforcement learning for bio-inspired navigation in complex environments
16:00–16:30	Coffee & Posters		
Chairman	Guillaume Baulieu		
16:30-16:55	CT	Kévin Bilaï Biloa iLM, Villeurbanne, France	Optimal navigation in fluctuating and disordered environments
16:55-17:20	CT	Isa B. I. Helal EC, Lyon, France	Reinforcement Learning for Non-Ideal Gas Turbulence Modeling
17:20-17:45	CT	Olivier Pierre-Louis iLM, Villeurbanne, France	Controlling the shape of fluctuating nanoscale clusters
17:45-18:10	CT	Kevin Alhada-Lahbab INL, Lyon, France	Reinforcement Learning-Assisted Ferroelectric Domain Wall Design Using a Machine Learning Phase-Field Surrogate

Thursday, 5 of June

Chairman	Gaël Tran		
9:00 – 10:00	IS	Kevin Maik Jablonka Jena, Germany	Encoding and Decoding Chemistry with Language Models
10:00–10:30	CT	Fabien Torralba ISA, Villeurbanne, France	On the classification of ¹ H NMR plants spectra(at an industrial scale)with a combined machine learning and metabolomic approach
10:30–11:00	Coffee		
Chairman	Olivier Stézowski		
11:00-11:30	IS	Corentin Herbert ENS, Lyon, France	Machine Learning for Extreme Climate Event Prediction
11:30-12:00	CT	Jérémie Dudouet IP2I, Villeurbanne, France	Analysing scanning tables data using neural networks
12:00-12:30	CT	Ugo Martinez Ecole Centrale, Lyon, France	Street-Scale Urban Air Temperature Prediction Using Citizen Weather Stations for Informed Urban Planning

List of posters

Quentin Pessemesse, * Marie-Ève Perrin, Pierre-Adrien Payard, Rodolphe Jazzar	ICBMS , Lyon, France	Quantifying the Electrophilicity of Carbenes by Linking Solid-State Nuclear Magnetic Resonance and Computational Descriptors
Mingjun Gu; Carine Michel, Stephan N. Steinmann	ENS Lyon, France	Electrostatically Embedded QM/MM Study of the Potential-Dependent Reorientation of Pyridine on Au(111)
R. Bachelet *, C. Furgeaud, M. Bounab, T. Zhu, C. Botella, P. Regreny, R. Rousseau, G. Saint-Girons	INL, Lyon, France	Towards smart growth of functional oxides with on-demand properties?
A. O. Afolabi*, C. Marichy, C. Journet, C. Bousige	LMI, Lyon, France	Synthesis of Boron-rich BxC Thin film via Chemical Vapor Deposition
P. Grigorev*, T. D. Swinburne, J. R. Kermode	MATEIS, Lyon, France	Use of foundation model for defects in BCC metals
J. Boulos*, V. Eglin , B. Kerautret , E. Larue , JM. Côme	LIRIS, Lyon, France	Image processing and deep learning for the characterization of polluted soils and their petrophysical properties

List of Abstracts – Talks

Bases, concepts, enjeux et limites de l'IA, dans la Science, pour soi et dans la société.

Jean-Luc Parouty CNRS / SIMaP

SIMaP - 1130 Rue de la Piscine - 38402 Saint Martin d'Hères – France

En l'espace de quelques années, l'intelligence artificielle – en particulier le Deep Learning – a connu des avancées remarquables, devenant capable de réaliser de nombreuses tâches auparavant réservées aux humains.

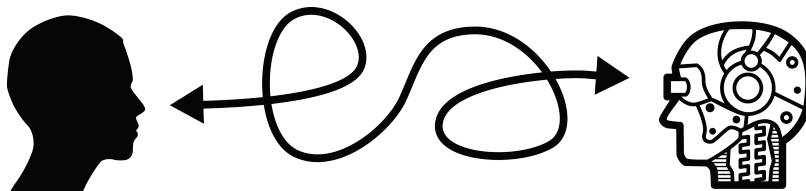
Entre fascination, scepticisme et inquiétude, ces progrès suscitent autant d'enthousiasme que de questionnements.

Cette présentation propose de retracer l'évolution de l'IA et du Deep Learning, d'en exposer les fondements théoriques, et d'offrir des repères concrets pour en faciliter la compréhension, l'exploration et l'appropriation. Des exemples appliqués à la science des matériaux viendront illustrer ces propos.

Un panorama des principaux acteurs de l'IA en France, ainsi que des ressources disponibles, sera également présenté.

Enfin, cette intervention mettra en lumière les limites actuelles de ces technologies, ainsi que les enjeux et impacts qu'elles soulèvent, qu'ils soient sociétaux, humains ou liés à la sécurité.

Le séminaire sera donné en français, mais les supports seront en anglais.



Keywords: IA, Deep Learning, Science, Impacts, Limites.



Jean-Luc Parouty, Ingénieur de Recherche CNRS au sein du laboratoire SIMaP.

Membre du cluster MIAI.

Spécialiste en l'IA et coordinateur de la formation/chaine FIDLE.

<https://www.youtube.com/c/CNRSFormationFIDLE>

Fueling the Digital Chemistry Revolution with Language and Multimodal Foundation Models

Teodoro Laino,^{1*}

¹IBM Research

*teo@zurich.ibm.com

One of the most important outcomes of organic chemistry is the creation of newly designed molecules. The application of domain knowledge gained through decades of laboratory experience has been critical in the synthesis of many new molecular structures. Nonetheless, most synthetic success stories are preceded by lengthy periods of unfruitful explorations. While automation systems proved exceptional in specific fields such as high-throughput chemistry, their use in general-purpose workflows remains a highly complex task, requiring the development of always unique software codifying distinct types of chemical operations. The digital revolution in chemistry hopes to streamline the adoption of digital models and automation with the use of data.

In the last years, natural language processing models have emerged as one of the most effective, scalable approaches for capturing human knowledge and modelling chemical processes in organic chemistry. Its use in machine learning tasks demonstrated high quality and ease of use in problems such as predicting chemical reactions [1-2], retrosynthetic routes [3], digitizing chemical literature [4], predicting detailed experimental procedures [5], designing new fingerprints [6] and yield predictions [7]. In this talk, I'll talk about the use and impact of language and multimodal foundation models in chemistry by highlighting the critical role of NLP architectures in implementing the first cloud-based AI-driven autonomous laboratory [8] and the use of visual transformer for implementing an efficient data capturing scheme.

References:

- [1] IBM Research Europe, *Chem. Sci.*, 2018, **9**, 6091-6098
- [2] IBM Research Europe, *ACS Cent. Sci.* 2019, **5**, **9**, 1572-1583
- [3] IBM Research Europe, *Chem. Sci.*, 2020, **11**, 3316-3325
- [4] IBM Research Europe, *Nat. Comm.*, 2020, **11**, 3601
- [5] IBM Research Europe, *Nat. Comm.*, 2021, **12**, 2573
- [6] IBM Research Europe, *Nat. Mach. Intel.*, 2021, **3**, 144–152
- [7] IBM Research Europe, *Mach. Learn.: Sci. Technol.*, 2021, **2**, 015016
- [8] <https://rxn.res.ibm.com>
- [9] IBM Research Europe, *Digital Discovery*, 2025



Teodor Laino received the Master degree in theoretical chemistry in 2001 (University of Pisa and Scuola Normale Superiore di Pisa, Italy) and the doctorate in computational chemistry in 2006 (Scuola Normale Superiore di Pisa, Italy) defending a thesis on 'Multi-Grid QM/ MM Approaches in ab initio Molecular Dynamics' supervised by Prof. Dr. Michele Parrinello. From 2006 to 2008, Teo worked as a post-doctoral researcher in the research group of Prof. Dr. Jürg Hutter at the University of Zurich, contributing to the development of the CP2K simulation package. In 2008, Teo joined the IBM Research - Zurich Laboratory (ZRL) as Research Scientist. He is currently Distinguished Research Scientist and manager.

His research interests focus on developing machine learning/artificial intelligence technologies to digitalize chemistry and materials science, with [IBM RXN for chemistry](#) being an example of a recent community success. In 2022, the team received the Sandmeyer Award of the Swiss Chemical Society for the important contributions to the field of digital chemistry.

Four Generations of Neural Network Potentials

Jörg Behler

Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, Germany
and

Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In recent years, there has been tremendous progress in the development of machine learning potentials (MLP) employing many different approaches [1]. Neural network potentials (NNPs), which have been introduced more than two decades ago, are an important class of MLPs. In general, MLPs can be classified into different generations representing their evolution with respect to applicability and physical phenomena they are able to describe. While the first generation of MLPs has been restricted to small molecules with only a few degrees of freedom, the second generation extended their applicability to high-dimensional systems containing thousands of atoms by constructing the total energy as a sum of environment-dependent atomic energies [2]. Long-range electrostatic interactions can be included in third-generation MLPs employing environment-dependent charges [3], and in the following years this locality approximation could be overcome by the introduction of fourth-generation MLPs [4,5], which are able to describe non-local charge transfer using a global charge equilibration step. In this talk an overview about the rapid evolution of high-dimensional NNPs will be given along with typical applications in chemistry and materials science.

- [1] J. Behler, J. Chem. Phys. **145** (2016) 170901.
- [2] J. Behler and M. Parrinello, Phys. Rev. Lett. **98** (2007) 146401.
- [3] N. Artrith, T. Morawietz, J. Behler, Phys. Rev. B **83** (2011) 153101.
- [4] S. A. Ghasemi, A. Hofstetter, S. Saha and S. Goedecker, Phys. Rev. B **92** (2015) 045131.
- [5] T. W. Ko, J. A. Finkler, S. Goedecker, J. Behler, Nature Comm. **12** (2021) 398.

Keywords: Machine Learning Potentials, Molecular Dynamics, Potential Energy Surface

Biography :



Jörg Behler graduated in chemistry at the University of Dortmund in 2000. In 2004 he obtained his PhD at the Fritz-Haber-Institute in Berlin. After a postdoctoral stay at the ETH Zürich, in 2007 he established his own research group at the Ruhr-Universität Bochum funded by a Liebig, an Emmy Noether and a Heisenberg fellowship. In 2013 he received the Hans G. A. Hellmann award for his work on the development of high-dimensional neural network potentials. In 2017 he became a full professor for theoretical chemistry at the University of Göttingen. In 2022 he returned to Bochum for a research professorship at the newly founded Research Center Chemical Sciences and Sustainability and for establishing a new Chair for Theoretical Chemistry II. His main research interest is the development and application of machine learning potentials in chemistry and materials sciences.

TRIP effect in Zirconia: atomistic simulations using neural network interatomic potentials

T. Albaret* ; G. Huynh ; J.-Y. Zhang ; M. Demetrio de Magalhaes ; D. Rodney

*Corresponding author

Institut Lumière Matière, Université Claude Bernard Lyon 1, Villeurbanne, France

MATEIS, INSA Lyon, Villeurbanne, France

tristan.albaret@univ-lyon1.fr

We developed and validated neural network interatomic potentials (NNP) using the DeepMD package to describe the complex polymorphism of zirconia and especially its mechanical properties related to transformation-induced plasticity (TRIP).

Zirconia ceramics, like steels, can undergo the TRIP effect through a phase transformation between tetragonal and monoclinic structures. Despite this similarity, the underlying mechanisms in zirconia remain incompletely understood. The potential was designed to capture for the first time the polymorphic behavior of both pure zirconia and its Ceria alloys. We simulated pillar compressions, with results compared to in situ Laue diffraction experiments. The simulations indicate a complex competition among stable and metastable phases, including several that have not yet been reported experimentally. This observation prompts further investigation into whether these phases are absent in experiments due to conditions such as sample size, temperature, strain rate, or boundary effects, or whether they reflect limitations inherent to the modeling approach.

Keywords: NNP Machine Learning Potential, Zirconia; Molecular dynamics; Martensitic transformation.

High-dimensional neural network potential for borophene on metallic surfaces

Colin BOUSIGE¹, Pierre MIGNON², Abdul-Rahman ALLOUCHE²

¹ Laboratoire des Multimatériaux et Interfaces, CNRS, Université Lyon 1, Villeurbanne, France

² Institut Lumière Matière, Université Lyon 1, Villeurbanne, France

colin.bousige@cnrs.fr

Single layer materials have drawn a lot of attention due to their peculiar physical properties (opto-electronic properties, high conductivity, flexibility...). In particular, it has been predicted that boron could exist as a single atomic layer in distinctive crystallographic configurations (allotropes), called *borophene* – in reference to the carbon equivalent, graphene. Borophene is one of the only 2D material with metallic behaviour, among other interesting properties [1]. Recent studies have focused on the synthesis of such material under various allotropic forms, the obtained allotrope depending on the substrate used and experimental parameters such as synthesis temperature [2–5]. However, the link between the various synthesis parameters and the obtained allotrope is still unclear. To be able to control the synthesis of allotropes selected for their wanted properties, one needs a good understanding of the growth mechanisms and phase transitions at stake in this system. Therefore, a strong theoretical support is needed, with accurate reactive simulations of large systems. However, while ab initio simulations are accurate, they are slow and do not allow studying large systems – and classical Molecular Dynamics require a force field that is not available for this system.

In this work [6], we have developed a new atomic potential using a machine learning approach [7–9], which allows us to explore multiple structural arrangements of borophene allotropes on metal substrates. The developed potential presents the advantage of performing fast simulations with a level of accuracy comparable to ab initio calculations [10]. Here, we will present the methodology to develop this machine learning potential as well as the various borophene allotropes that have been simulated on Ag surfaces, and present our first results on the growth and phase transitions in this system using our machine learned potential.

References

1. Mannix et al., *Nat. Nanotech* **13** (2018), 444–450
2. Mannix et al., *Science* **350** (2015), 1513–1516
3. Kiraly et al., *ACS Nano* **13** (2019), 3816–3822
4. Feng et al., *Nat. Chem* **8** (2016), 563–568
5. M. Cuxart et al., *Sci. Adv.* **7** (2021), eabk1490
6. P. Mignon et al., *J. Am. Chem. Soc.* **145** (2023), 27857–27866
7. J. Behler & M. Parrinello, *Phys. Rev. Lett.* **98** (2007), 146401
8. J. Behler, *Int. J. Quantum Chem.* **115** (2015), 1032–1050
9. Singraber et al., *J. Chem. Theory Comput.* **15** (2019), 3075–3092
10. Singraber et al., *J. Chem. Theory Comput.* **15** (2019), 1827–1840

A Neural Network Atomistic Potential for Pyrophyllite Clay Simulations

C. SANZ¹, A-R. ALLOUCHE¹, C. BOUSIGE², P. MIGNON^{1*}

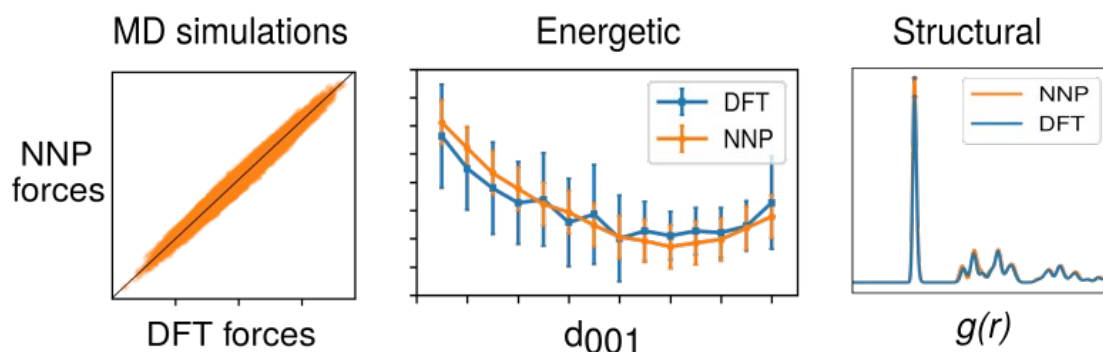
* Corresponding author

¹Institut Lumière Matière, UMR CNRS 5306, Université Claude Bernard Lyon 1, F-69100 Villeurbanne, France

²Laboratoire des Multimatériaux et Interfaces, UMR CNRS 5615, Université Claude Bernard Lyon 1, F-69100 Villeurbanne, France

E-mail : pierre.mignon@univ-lyon1.fr

Pyrophyllite clays ($\text{Al}_2(\text{Si}_4\text{O}_{10})(\text{OH})_2$) are dioctahedral minerals, with great adsorption capacity for a wide range of compounds, giving them possible applications in pollutants removal. We developed a neural networks potential (NNP) for pyrophyllite clay minerals, with the Behler-Parinello approach, using an adaptive learning scheme to construct our dataset. The obtained neural network potential was evaluated by comparing the results of molecular dynamics ran with our NNP to those obtained by DFT, classical force fields, and experimental results. The developed potential is able to reproduce structural parameters, among which the radial distribution functions $g(r)$, or basal spacing (d_{001}) energetic profile, with excellent agreement to experimental data. Other properties such as vibrational spectra, and exfoliation energy (the energy needed to peel off a single layer of a bulk structure) are also rather accurately reproduced. These results are very encouraging, as these are the first NNPs allowing the description of clay layers held together only by van der Waals interactions.



Keywords: neural network potential, atomistic simulation, clay minerals

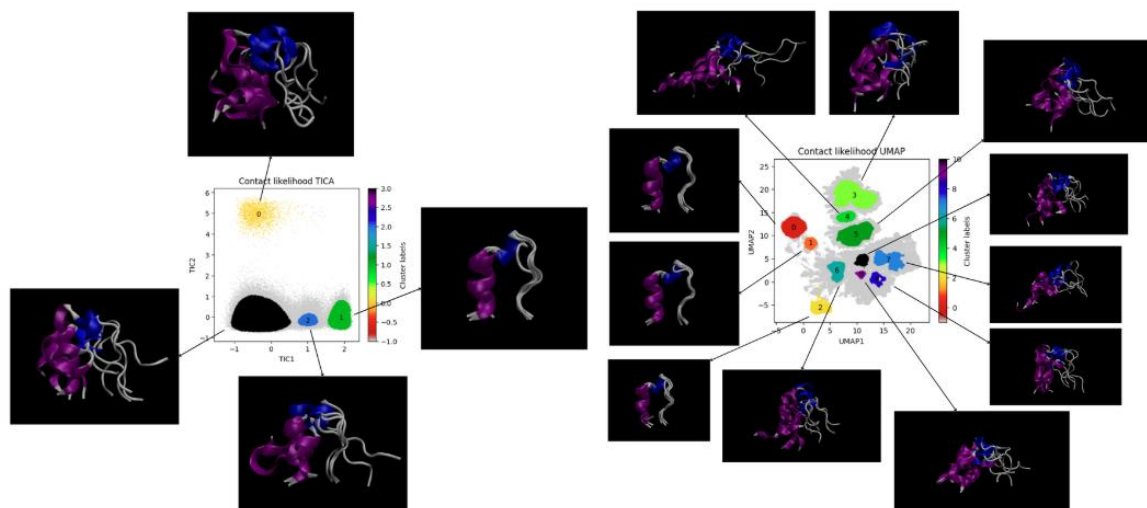
List of Abstracts – Talks

Identifying conformational states of TRP-Cage using dimensionality reduction and clustering methods

S.Jatiere; D.Bissuel ; C.Loison

Institute of Light and Matter, Université Claude Bernard Lyon 1, Villeurbanne, France
steve.jatiere@univ-lyon1.fr

Proteins dynamics is essential to their function. Molecular dynamics (MD) simulations are routinely employed to study protein conformational changes. Theoretically, Markov State Model (MSM) can extract representative conformations from MD trajectories and describe the kinetics of transitions between them. In this work, we shall compare dimensionality reduction techniques with machine learning algorithms, using case study proteins, such as the small TRP-cage. We compare several molecular descriptors-including cartesian coordinates, α distances, dihedral angles, and contact likelihoods as input features. These features are then embedded into low-dimensional spaces using various dimensionality reduction techniques such as PCA (Principal Component Analysis), TICA (Time-lagged Independent Component Analysis), UMAP (Uniform Manifold Approximation and Projection), and VAE (variational autoencoders), see Figure below. Clustering algorithms including k-means, HDBSCAN (Hierarchical Density-Based Spatial Clustering of Application with Noise), and Gaussian Mixture Models are applied to reveal metastable states. Beyond benchmarking these approaches, we aim to assess whether UMAP offers a more effective representation of the conformational landscape for building accurate MSM.



Clustering of the TRP-cage protein conformations after two different 2D-dimensionality reductions: TICA (left) and UMAP (right). The initial features were 190 native contact likelihood of the Ca-Ca distances. The clustering was done with HDBSCAN.

Keywords: Molecular dynamics; Dimension reduction; Clustering; Markov State Model; Protein conformation.

List of Abstracts – Talks

Mechanism of Ag⁺-induced folding of a bacterial peptide from molecular dynamics simulations and deep dimensionality reduction

Florian E.C. Blanc ^{a,*}, Maggy Hologne ^a, Henry Chermette ^a, Mélodie Demontrond ^a, Olivier Walker ^{a,*}

^a Université de Lyon, CNRS, UCB Lyon1, Institut des Sciences Analytiques, UMR5280, Villeurbanne, France

*Correspondence: florian.blanc@isa-lyon.fr, olivier.walker@univ-lyon1.fr

Metal cations shape the conformational landscapes of proteins in various ways. As a remarkable example, the intrinsically disordered protein SilE folds into α -helical segments upon binding Ag⁺ ions, but the details of this process are still unclear. Focusing on the 11-residue B1 peptide fragment from SilE, we investigate here the mechanism of Ag⁺-induced folding into an α -helix at atomic resolution using Molecular Dynamics (MD) simulations and deep learning. We sampled the conformational space of B1 in the absence and the presence of Ag⁺ using temperature replica-exchange MD simulations (C36m force-field, 78 μ s aggregate simulation time). We computed free energy landscapes along bespoke collective variables, including latent variables learnt with an autoencoder (AE) neural network. This enabled us to map B1's conformational landscape and how it is shaped by Ag⁺. We then characterized the folding pathways of B1 with an original string method-based strategy. We find that Ag⁺ binding shifts the equilibrium toward the α -helical form (in agreement with experimental observations) and alters the folding mechanism by stabilizing different intermediates. In addition, the AE-learned variables reveal off-pathway metastable conformers, some of which are destabilized by Ag⁺. Overall, we describe an original case of metal-induced folding and showcase how autoencoders help map complex conformational landscapes from atomistic simulations.

Keywords: Atomistic simulations; Deep autoencoders; Free energy; Peptide folding; Metal-protein interactions

Physics-informed and augmented learning in fluids and solid mechanics

Beatriz MOYA

Arts et Métiers Institute of Technology, Paris

CNRS@CREATE, Singapore

Beatriz.moya_garcia@ensam.eu

Artificial Intelligence (AI) in general, and Machine Learning (ML) in particular, represent appealing routes in science, engineering and technology. However, in many domains of science and engineering, a huge amount of knowledge exists in form of data, domain expert knowledge and models based on physics and chemistry. In these cases, allying the existing knowledge with the online collected data, within the so-called hybrid paradigm, represents an appealing route to empower engineering and technology.

Thus, the use of informed machine learning enables accurate and real-time simulations of physics-based models, based on the construction of surrogates from high-fidelity physics-based simulations. Moreover, informed machine learning enables modelling the prediction-to-measures gap, enabling enriching (or correcting) physics-based models within the so-called hybrid paradigm. As ML is only used to model the gap, the amount of required data reduces significantly, with the associated energy and environmental imprint. This hybrid framework makes also possible addressing larger systems, involving complexity and uncertainty, while explaining hybrid models predictions and decisions. In such framework, thermodynamics is an appealing bias to impose physically grounded constraints that enhance model generalization, stability, and consistency with real-world behavior.

Thus, informed machine learning enables predicting faster, better (accuracy), cheaper, larger, safer, ... crucial in engineering operations. However, engineering many times addresses design, and then, only historical or synthetic data can be employed. In the domain of engineering design, AI can help to make different, by generating optimal designs with respect to the concerned quantities of interest. The so-called generative AI is at the heart of generative design, and has been successfully applied to chemicals, designs, materials, processes, ... enlarging and optimizing engineering outcomes.



Beatriz Moya received her MSc Eng. and PhD in Mechanical Engineering from the University of Zaragoza, Spain. She was awarded a Margaritas Salas – EU Next Generation fellowship in 2022 and became Research fellow in the project DesCartes at CNRS@CREATE, Singapore, for the study of smart cities in 2023. Currently, Beatriz is Associate Professor and Junior Chair at the PIMM laboratory in École National Supérieure d'Arts et Métiers, Paris, working on the strategy of interpretable AI informed by physics and its synergy with the hybrid modeling paradigm. She is also the Project Manager and director of the Centre Michel Serres program for interdisciplinary studies, and editor of the international journal AMSES. Her research strives for the use of hybrid modeling in engineering applications such as structural health monitoring or dynamical modeling performing an interdisciplinary combination of computer vision techniques and physics informed artificial intelligence. She is currently the president of the young section of the Spanish Association in Computational Mechanics (SEMNI) and committee member of the young researchers' chapter of ECCOMAS (EYIC).

Bayesian Optimization for chemical research

Víctor Sabanza-Gil

École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

victor.sabanzagil@epfl.ch

Bayesian Optimization (BO) has recently become a useful tool to guide chemical research and find optimal conditions or candidates in a sample-efficient way [1][2]. In this talk, we will first introduce the key concepts in BO and its practical implementation in the experimental chemistry domain [3]. We will then discuss current research trends in the field, remarking our last work in multi-fidelity BO [4], and how large-language models can be used to improve the optimization results. Overall, we want to provide practical insights about the use of BO in real chemical problems and show its usefulness in daily optimization scenarios.

Keywords: bayesian optimization, chemistry, multi-fidelity

References

- [1] J. Guo, B. Ranković, P. Schwaller, “Bayesian Optimization for Chemical Reactions”, *Chimia* **2023**, 77, 31
- [2] B.J. Shields, J. Stevens, J. Li, et al. “Bayesian reaction optimization as a tool for chemical synthesis.” *Nature* **2023**, 590, 89–96
- [3] T. Cinquin, S. Lou, F. Strieth-Kalthoff, et al. “What actually matters for materials discovery: pitfalls and recommendations for Bayesian Optimization”. *AI 4 Materials workshop, ICLR 2025*
- [4] V. Sabanza-Gil, R. Barbano, D. Pacheco Gutiérrez, J. S. Luterbacher, J. M. Hernández-Lobato, P. Schwaller, L. Roch. “Best Practices for Multi-fidelity Bayesian Optimization in Materials and Molecular Research” - *NeurIPS 2024 Workshop on AI for New Drug Modalities*

Process Analytical Technology (PAT) at polyolefin recycling service: real-time monitoring using *in-situ* spectroscopy and chemometrics

S. Ferchichi^a, N. Sheibat-Othman^b, M. Rey-Bayle^a, V. Monteil^{c*}

* Corresponding author

^aIFP Energies Nouvelles, Rond-Point de l'échangeur de Solaize, 69360 Solaize, France

^bUniversite Claude Bernard Lyon 1, LAGEPP, UMR 5007 CNRS, 69622 Villeurbanne, France

^cUniversite Claude Bernard Lyon 1, CP2M, UMR 5128, CNRS, 69616 Villeurbanne, France

vincent.monteil@univ-lyon1.fr

In the past thirty years, significant efforts have been dedicated to the recycling of waste plastics. This is motivated by the increased collective awareness and concerns about the environmental impact of plastics, besides economic benefits. From the different recycling techniques, solvent-based recycling is the most promising because it offers the possibility to recover a virgin polymer from plastic waste, free of all additives like fillers or pigments. The obtained polymer can possibly be reused in the same or different applications than its original use.

We proposed to monitor different parameters during the different steps involved in the recycling process using *in situ* spectroscopy analysis such as the dissolved polymer content, polymer degradation, or additive content. When combined with chemometrics, these powerful tools appear to be very useful for the monitoring and successful completion of recycling processes. Indeed, we developed a methodology which allows to monitor in real time the dissolved concentration of polypropylene plastic charges in several types of solvents, solvent mixtures and solvents not used during the model development.

Keywords: Polypropylene, Chemometrics, Recycling, PLS, Monitoring

Approximation of mean curvature flows by an interpretable data-driven neural network

Élie Bretin* ; Roland Denis ; Simon Masnou ; Garry Terii

* Corresponding author

Univ Lyon, Institut Camille Jordan, CNRS UMR 5208, Institut Camille Jordan, 43 bd. du

11 novembre 1918

elie.bretin@insa-lyon.fr

I will first describe a simple neural network able to learn the (isotropic) mean curvature flow of oriented interfaces (i.e., boundaries of domains). Its structure draws inspiration from splitting schemes used for the discretization of the Allen-Cahn equation, which approximates the mean curvature flow of domain boundaries using a phase field representation. Despite its simplicity and the fact that it is trained only on evolving disks, this neural network is accurate and demonstrates excellent generalization to more complex geometric shapes. Slightly more complex networks, recursively designed from the initial structure, appear to handle also non-oriented interfaces, for which no efficient phase-field model was previously known. They can also handle singularities such as triple points. The approach can be generalized to handle the case of anisotropic surface energies and can be coupled with additional constraints to extend their applications: volume constraint, multiphase case, inclusion constraints for Steiner or minimal surfaces. The networks simplicity is of interest from an interpretability point of view: the structure of the network designed for the non-oriented case has made it possible, a posteriori, to identify an equation that models this flow, and once trained on the data, the Wulff shape can be easily extracted from the network's coefficients, even in the case of anisotropic surface energies.

Keywords: mean curvature flow, phase field, neural network, interpretability, anisotropy.

Metainterfaces with specified friction laws : new designs from numerical optimization

L. Fu^{*}, D. G. Kashala, D. Dalmas, J. Scheibert^{*}

Laboratoire de Tribologie et Dynamique des Systemes, École Centrale de Lyon, CNRS,
Lyon, France

li.fu@ec-lyon.fr, julien.scheibert@ec-lyon.fr

Many devices, including touchscreens and robotic hands, involve frictional contacts. Optimizing these devices requires fine control of the interface's friction law. We have recently proposed a generic surface design strategy to prepare dry rough interfaces that have predefined relationships between normal and friction forces [1]. Such metainterfaces are based on assemblies of spherical asperities, whose individual heights are prescribed through inversion of a suitable upscaling model. In [1], the inversion was analytical, which strongly limited the number of accessible friction laws. Here, we use genetic algorithms to identify complex designs that meet previously inaccessible specifications. We apply this method to obtain friction laws with a true proportionality between friction and normal forces at large normal forces. This method therefore offers ways to create metainterfaces with on-demand values of the friction coefficient, without changing the pair of materials in contact. Our new designs are validated experimentally on glass/polydimethylsiloxane (PDMS) metainterfaces. Overall, these results pave the way for automated ways of designing soft contact interfaces with virtually any desired friction behavior.

Keywords: metainterface, tribology, optimization, genetic algorithm

How unsupervised machine learning can provide benchmark input for nanoalloy design

Matthias Hillenkamp^{1,2*}, Murilo Moreira^{1,2}, Emmanuel Cottancin¹, Michel Pellarin¹, Lucian Roiban³, Karine Masenelli-Varlot³, Daniel Ugarte², Varlei Rodrigues²

¹ Institute of Light and Matter, University Lyon, University Claude Bernard Lyon 1, CNRS, UMR5306; Villeurbanne F-69622, France.

² Institute of Physics Gleb Wataghin, State University of Campinas; Campinas, SP, 13083-970, Brazil.

³ INSA Lyon, University Claude Bernard Lyon 1, CNRS, MATEIS, UMR5510; 69621 Villeurbanne, France.

Bimetallic nanoparticles (BNPs) are used in numerous applications in catalysis, plasmonics or fuel cell technology. The addition of the second metal to the nanoparticles allows enhancing and fine-tuning their properties by choosing their composition, size, shape and environment. However, the crucial additional parameter of chemical structure within the particle is difficult to predict and access experimentally, even though segregated core-shell structures and random alloys can have drastically different physicochemical properties. This is highlighted by the vast literature on the most studied bimetallic system, gold-silver, for which the controversy on whether gold and silver are miscible on the nanoscale or segregate persists. As long as simulations are not able to correctly reproduce the elemental structure of nanoscale systems, any predictions of properties remain equivocal.

This presentation shows how unsupervised machine learning (PCA and NMF), performed on experimental X-ray spectroscopy data for relaxed and surfactant-free AgAu BNPs, can help provide reliable benchmark input for the validation of complex materials design simulations such as neural networks.

Moreira *et al.* Small 2411151 (2025), <https://doi.org/10.1002/sml.202411151>.

Keywords: Nanoalloys, unsupervised machine learning, electron microscopy (STEM-EDX), PCA, NMF

List of Abstracts – Talks

Deep Scopie: an introduction to machine learning for imaging

David Rousseau ; david.rousseau@univ-angers.fr

Université d'Angers, LARIS, UMR INRAe IRHS, Angers, France.

We introduce machine learning (both shallow and deep learning) in the context of imaging. We specifically address challenges related to computational imaging where the raw acquisition requires processing before being interpretable by humans or machines. We illustrate this topic with various applications such as denoising, super-resolution, inverse problems, multimodal imaging, smart scanning... We will discuss the opportunities and challenges of bridging the model-based physics of imaging with a purely data-driven approach. The talk will be illustrated with a wide range of imaging modalities such as computed tomography imaging spectrometer [1], fluorescent microscopy [2], Raman microscopy [3], X-Ray tomography [4], RGB-Depth imaging [5].

David Rousseau serves as professor of data science in the physics department at the Université d'Angers, where he leads the Imaging for Horticulture and Phenotyping team.

A selection of recent publications on the topic by the speaker:

- [1] Douarre, C., Crispim-Junior, C. F., Gelibert, A., Germain, G., Tougne, L., & Rousseau, D. (2021). CTIS-Net: a neural network architecture for compressed learning based on computed tomography imaging spectrometers. *IEEE Transactions on Computational Imaging*, 7, 572-583.
- [2] Ahmad, A., Sala, F., Paiè, P., Candeo, A., D'Annunzio, S., Zippo, A., ... & Rousseau, D. (2022). On the robustness of machine learning algorithms toward microfluidic distortions for cell classification via on-chip fluorescence microscopy. *Lab on a Chip*, 22(18), 3453-3463.
- [3] Gilet, V., Mabilieu, G., Loumaigne, M., Coic, L., Vitale, R., Oberlin, T., ... & Rousseau, D. (2023). Superpixels meet essential spectra for fast Raman hyperspectral microimaging. *Optics Express*, 32(1), 932-948.
- [4] Hamdy, S., Charrier, A., Corre, L. L., Rasti, P., & Rousseau, D. (2024). Toward robust and high-throughput detection of seed defects in X-ray images via deep learning. *Plant Methods*, 20(1), 63.
- [5] F. Mercier, G. Couasnet, A. El Ghaziri, N Bouhlel, A Sarniguet, M Marchi, M Barret, D Rousseau. Deep-learning-ready RGB-Depth images of seedling development. *Plant Methods* (in press 2025)

Youtube channel : <https://www.youtube.com/@imhorphenbioimagingrearc95>

Keywords: Computational imaging ; Compressed sensing, Deep learning.

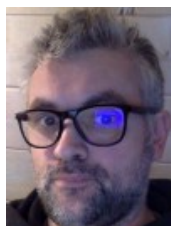


Image processing and deep learning for the characterization of polluted soils and their petrophysical properties

J. Boulos^{1,3*}; V. Eglin¹; B. Kerautret²; E. Larue³; JM. Côme³

¹Université de Lyon, INSA-Lyon, LIRIS, UMR 5205, 69100, Lyon, France

²Université de Lyon, Lyon 2, LIRIS, UMR 5205, 69100, Lyon, France

³Ginger BURGEAP, Département R&D, 69425, Lyon, France

*j.boulos@groupeginger.com

In France, over 350000 sites are potentially polluted, including 60000 in Auvergne-Rhône-Alpes. Most of these sites are contaminated by organic liquid contaminants, such as hydrocarbons and PCBs (Polychlorobiphenyls). The current method of pollution diagnosis, based on soil sampling, is costly and time-consuming. Moreover, this method frequently leads to errors in the assessment of pollutants and volumes of contaminated soil, impacting on the choice of remediation techniques, the cost and duration of treatments. To this end, GINGER R&D team aims to develop an in-situ image processing technique for estimating pollution and soil petrophysical properties, providing near-real-time quantitative data. In this context, a classification model based on embeddings generated by neural networks is being developed, making it possible to exploit multiple descriptors such as color, and those derived from neural embeddings. These descriptors will be computed on a variety of modalities, including color images and from different acquisition sources. This deep learning model, developed from a database created during the thesis, will be evaluated on several levels: controlled-condition images, cubitainer data and data from real sites. In this work, we present our initial results obtained by fine-tuning a pre-trained model to classify images into lithological classes and water saturation levels, enhancing polluted site characterization and remediation efforts.

Keywords: Image Processing, Deep Learning, Petrophysical Properties, Polluted Soil Diagnosis.

Small, hand-designed Convolutional Neural Networks for biomedical image analysis

O. Cochet-Escartin*, L. Combe, A. Chambost, S. Monnier, H. Delanoë-Ayari

* Corresponding author

Institut Lumière Matière, 10 rue Ada Byron, Villeurbanne

Olivier.cochet-escartin@univ-lyon1.fr

Convolution Neural Networks (CNNs) have revolutionized the field of computer vision in the last decade. In biophysics, quantitative image analysis has a predominant role in extracting relevant data from, for example, microscopy images. However, developing these models requires choosing many important parameters related to their precise architecture or to how they should be trained. As these choices can seem difficult to the untrained eye, a common alternative is transfer learning which uses pre-existing CNNs and fine-tunes them for the task at hand with limited knowledge required. In this talk, through two practical examples from biophysics, I will show how and why small, hand-designed CNNs are often preferable to transfer learning and, in the process, provide a set of basic rules which can help researchers efficiently develop their own CNNs to address their image analysis problems.

Keywords: Computer vision, CNNs, microscopy, biophysics.

LIBS hyperspectral imaging with AI: a strong analytical potential

Vincent Motto-Ros¹, Ludovic Duponchel²

¹*Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, 69622 Villeurbanne, France*

²*Laboratoire de Spectroscopie pour les Interactions, la Réactivité et l'Environnement, LASIRE, CNRS UMR 8516, Université de Lille, Faculté des Science et Technologies, 59655, Villeneuve d'Ascq, France*

vincent.motto-ros@univ-lyon1.fr

High-sensitivity elemental imaging remains a major technological challenge, typically relying on complex and specialized systems such as synchrotron X-ray fluorescence (SXRF) or laser ablation coupled with inductively coupled plasma mass spectrometry (LA-ICP-MS). Our team has developed an innovative, fully optical, fast, and accessible multi-elemental imaging technique. Based on Laser-Induced Breakdown Spectroscopy (LIBS), this approach enables the mapping of elements from the periodic table in virtually any type of solid sample — including biological tissues, rocks, and industrial materials — with sensitivity down to the ppm level and spatial resolution around 10 μm [1,2].

Despite its potential, LIBS imaging faces significant challenges when it comes to data analysis. The inherent spectral complexity and the massive volume of data produced make this step both time-consuming and demanding. Depending on the spatial resolution, datasets can easily reach several tens of gigabytes per sample. Moreover, each spectrum is acquired from a single laser shot and may therefore be quite noisy. The need to process a large number of complex and noisy spectra introduces recurring issues that can affect image quality — including spectral interferences, inaccurate signal extraction, and potential information loss. In this presentation, we will highlight the main obstacles encountered during the data processing stage. We will then explore various methods for constructing elemental images from spectral datasets, ranging from basic peak intensity extraction to advanced approaches based on artificial intelligence. A particular focus will be placed on the capabilities and advantages of AI in this context.

- [1] B. Busser, S. Moncayo, J.-L. Coll, L. Sancey, V. Motto-Ros, Elemental imaging using laser-induced breakdown spectroscopy: A new and promising approach for biological and medical applications, *Coordination Chemistry Reviews* 358, 70-79 (2018).
- [2] L. Jolivet, M. Leprince, S. Moncayo, L. Sorbier, C.-P. Lienemann, V. Motto-Ros, Review of the recent advances and applications of LIBS-based imaging, *Spectrochim. Act. B* 151, 41-53 (2019).

Convolutional Neural Network trained with Attenuated Total Reflectance for hydroxyl quantification in lignin

Hugo Lilti*, Ruben Checa, Christophe Geantet, Dorothée Laurenti
Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256 – CNRS /
Université Lyon 1
hugo.lilti@ircelyon.univ-lyon1.fr

The quantification of hydroxyl groups in lignin is crucial for understanding its reactivity and potential applications in biomaterials as a renewable alternative to fossil-based polyols. This study presents a robust method for quantifying hydroxyl groups using Attenuated Total Reflectance Infrared Spectroscopy (ATR-IR) which offers an easy and fast analytical approach. To do so we trained a Convolutional Neural Networks (CNNs) to predict hydroxyls moieties measured by ^{31}P Nuclear Magnetic Resonance (NMR) using only ATR-IR spectra, providing an accurate and easy way of quantitatively analyzing complex spectral data. The results demonstrate that the CNN-based method shows a good precision and reliability to quantify hydroxyl group compared to traditional chemometrics methods such as Partial Least Square regression. Notably, this method is robust across different lignin type and origin, including Soda, Kraft, Organosolv and both softwood and hardwood. This study illustrates that performing quantitative analysis of lignin (and biomass in general) can be significantly facilitated using machine learning. Future work will focus on expanding this method to other functional groups, inter-unit bond, molecular masses and other biopolymers. The development of in-situ measurements during biomass conversion process could also be considered.

Keywords: Biomass, CNN, ATR-FTIR, Lignin

Reinforcement Learning:

Aurélien Garivier
Ecole Normale Supérieure de Lyon
aurelien.garivier@ens-lyon.fr

Reinforcement Learning (RL) offers a powerful framework for sequential decision-making under uncertainty, with some spectacular successes in the recent decade and a growing impact in the physical sciences. In this talk, we present the core principles of RL and highlight its relevance to modern AI developments. We try to give a special focus on possible applications in chemistry and physics, such as molecular design or adaptive experimental control.

Reinforcement learning for bio-inspired navigation in complex environments

Aurore Loisy

Aix Marseille Univ, CNRS, Centrale Med, IRPHE, Marseille, France

Navigation is about optimising a route to go from A to B. Animal and robotic navigation however fundamentally differ from the routing of planes and ships, because it is autonomous : the self-propelled « agent » has only access to information from its own sensors to make decisions. This type of problem is well-suited for reinforcement learning, a branch of artificial intelligence which has gained popularity by beating human players at games. I will show how we can leverage modern (deep) reinforcement learning techniques to solve navigation problems inspired by the animal world, such as the vertical migration of plankton through the water column, the search for an odor source by insects, and chemical-guided collective foraging.

Keywords: reinforcement learning, partially observable Markov decision process, olfactory search, navigation in turbulent flows, bio-inspiration

Optimal navigation in fluctuating and disordered environments

K. Bilal Bilal ; O. Pierre-Louis *

* Corresponding author

Institut Lumière Matière, 10 rue Ada Byron 69100 Villeurbanne

olivier.pierre-louis@univ-lyon1.fr

Navigation encompasses a broad range of processes, from animal behavior to autonomous vehicles. In our research, we applied model-based reinforcement learning, known as Dynamic Programming, to derive optimal navigation strategies in complex environments. Our main objective is to explore how fluctuations and disorder affect these navigation strategies.

We use the general decision-making framework provided by Markov Decision Processes, where an agent in an environment has to find the optimal actions that minimize a specified cost. The chosen environment for this study is the classical gridworld problem, in which an agent performs a random walk on a square lattice and uses actions to bias its movement toward specific directions. The primary objective is for the agent to reach a target location in minimum time. Consequently, our problem involves finding the best set of actions, known as the optimal policy, that achieves this goal. We further extend our analysis to gridworld scenarios that include defects, examining and characterizing the optimal policies when one or multiple defects are present.

Keywords: Reinforcement Learning, Dynamic Programming, Navigation.

Reinforcement Learning for Non-Ideal Gas Turbulence Modeling

I. B. I. Helal^{1,2*}; A. Giauque¹; C. Corre¹; E. Sauret²

* Corresponding author

¹Ecole Centrale de Lyon, 36 avenue Guy de Collongue, 69130 Ecully, France

²Queensland University of Technology, 32 George St, Brisbane City QLD 4000, Australia
isa.helal@ec-lyon.fr

In order to save energy, recovering fatal heat is necessary. One way to do this is by using non-ideal gases as working fluids in dedicated thermodynamic cycles. However, current closure models for Reynolds-averaged Navier-Stokes fail to capture all the aspects of the turbulent behavior of non-ideal gases (see (Giauque et al., 2023) for example), due to their complex thermo-physical properties. The present work aims at improving Reynolds-averaged Navier-Stokes closure models using a Reinforcement Learning (RL) strategy. The soft actor-critic (SAC) algorithm (Haarnoja et al., 2018) is implemented and validated in the case of a turbulent flat plate; first for outlet skin friction control through manipulating the inlet turbulence intensity, then for obtaining a reference outlet turbulent viscosity profile by modulating the turbulent viscosity field in the domain. In our final contribution, the RL algorithm will be trained to match the $k-\omega$ SST turbulence model results by imposing the values of the model constants in a validation case selected from the NASA turbulence modeling testing challenge (Rumsey & Coleman, 2022).

Keywords: compressible turbulence modeling, reinforcement learning.

Controlling the shape of fluctuating nanoscale clusters

Olivier Pierre-Louis*, Francesco Boccardo

* Corresponding author

ILM-Lyon, UCB Lyon 1

olivier.pierre-louis@univ-lyon1.fr

We have investigated how one can manipulate the shape of a small cluster of colloids (or nano-particles) using an external field in the presence of thermal fluctuations [1, 2, 3]. This problem can be formulated as a minimization of first passage times in configuration space. We obtain the optimal solution using Dynamic Programming. We then show how the efficiency of Reinforcement-Learning approaches vanishes at the nanoscale due to thermal fluctuations [4].

Keywords: Reinforcement Learning ; Dynamic Programming ; First passage processes ; fluctuations.

[1] F Boccardo, O Pierre-Louis Physical Review Letters 128, 256102 (2022)

[2] F Boccardo, Y Benamara, O Pierre-Louis Physical Review E 106, 024120 (2022)

[3] F Boccardo, O Pierre-Louis Journal of Statistical Mechanics : T&E (10), 103205 (2022)

[4] F Boccardo, O Pierre-Louis Phys. Rev. E 110, L023301 (2024)

Reinforcement Learning-Assisted Ferroelectric Domain Wall Design Using a Machine Learning Phase-Field Surrogate

Kevin Alhada-Lahbabi, Damien Deleruyelle, Brice Gautier¹

1. INSA Lyon, CNRS, Ecole Centrale de Lyon, Université Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69622, Villeurbanne, France

Precise control of ferroelectric domain walls (DWs) is a pivotal challenge for advancing DW-based memory device technologies. While recent advancements in scanning probe microscopy-enabled automated experiments have improved the efficiency of tip control, real-time optimization of tip trajectories for configuring arbitrary domain structures remains a significant hurdle.

In this study, we propose a reinforcement learning (RL) framework for autonomous DW manipulation, employing a three-dimensional machine learning phase-field surrogate model to accelerate environment dynamics [1]. An overview of the proposed methodology is depicted in Figure 1, illustrating the agent's interaction with the environment to configure DWs via tip-induced switching. Initially, we explore a single-goal RL strategy, wherein the agent adjusts the DW configuration to match a specific DW target by controlling the tip's spatial position and applied bias on the film surface. Subsequently, we extend the approach with a goal-augmented RL strategy, enabling the agent to generalize across diverse target configurations and optimize tip trajectories in real time for arbitrary targets without requiring retraining. Furthermore, we demonstrate the agent's capability to design domain structures at the patch level, facilitating precise polarization control in large-scale systems. The framework is also adapted to directly optimize ferroelectric properties in an inverse design context rather than focusing on specific DW configurations. Collectively, this RL framework marks a substantial step forward in real-time design and control of ferroelectric DWs.

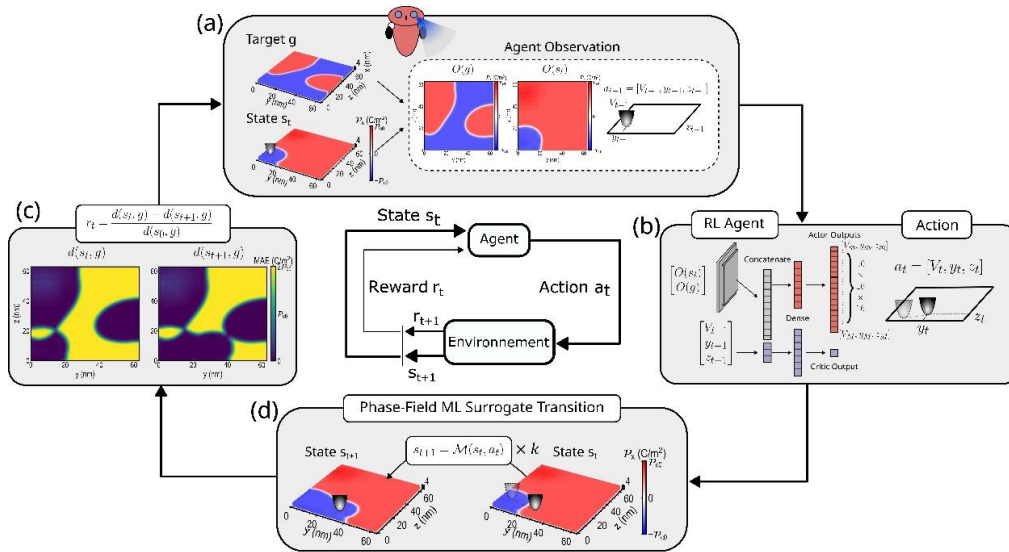


Figure 1. Overview of the RL Framework for Tip-Assisted Domain Wall Control. (a) At each timestep, the agent observes the environment (current state, domain wall target surface, prior action) and (b) selects an action consisting of tip offset and location ($a_t = [u_T, y_T, z_T]$). (c) A reward is then assigned based on the agent's progress toward achieving the target configuration, following the transition of the environment simulated by the machine learning-based phase-field surrogate model (d).

[1] Alhada-Lahbabi, K., Deleruyelle, D., Gautier, B. Machine learning surrogate for 3D phase-field modeling of ferroelectric tip-induced electrical switching. *NPJ Computational Materials* **10**, 197 (2024).

Encoding and Decoding Chemistry with Language Models

Kevin Maik Jablonka

Friedrich Schiller Universität Jena & Helmholtz Institute for Polymers in Energy Applications Jena

The field of chemical sciences has seen significant advancements with the use of data-driven techniques, particularly with large datasets structured in tabular form.

However, collecting data in this format is often challenging in practical chemistry, and text-based records are more commonly used [1]. Using text data in traditional machine-learning approaches is also difficult.

Recent developments in applying large language models (LLMs) to chemistry have shown promise in overcoming this challenge. LLMs can convert unstructured text data into structured form and can even directly solve predictive tasks in chemistry. [2, 3] In my talk, I will present the impressive results of using LLMs, showcasing how they can autonomously utilize tools and leverage structured data and “fuzzy” inductive biases.

To enable the training of a chemical-specific large language model, we have curated a new dataset along with a comprehensive toolset to utilize datasets from knowledge graphs, preprints, and unlabeled molecules. To evaluate frontier models trained on such a dataset, we specifically designed a benchmark to evaluate the chemical knowledge and reasoning abilities. I will present the latest results, demonstrating the potential of LLMs in advancing chemical research. [4]

References:

- [1] Jablonka, K. M.; Patiny, L.; Smit, B. *Nat. Chem.* 2022, 14 (4), 365–376.
- [2] Jablonka, K. M.; et al. *Digital Discovery* 2023, 2 (5), 1233–1250.
- [3] Jablonka, K. M.; Schwaller, P.; Ortega-Guerrero, A.; Smit, B. *Leveraging large language models for predictive chemistry.* *Nat. Mach. Int.* 2024, 6, 161–169.
- [4] Mirza, A.; Alampara, N.; Kunchapu, S.; Emoekabu, B.; Krishnan, A.; Wilhelmi, M.; Okereke, M.; Eberhardt, J.; Elahi, A. M.; Greiner, M.; Holick, C. T.; Gupta, T.; Asgari, M.; Glaubitz, C.; Klepsch, L. C.; Köster, Y.; Meyer, J.; Miret, S.; Hoffmann, T.; Kreth, F. A.; Ringleb, M.; Roesner, N.; Schubert, U. S.; Stafast, L. M.; Wonanke, D.; Pieler, M.; Schwaller, P.; Jablonka, K. M. *Are Large Language Models Superhuman Chemists?* *arXiv* 2024. <https://doi.org/10.48550/ARXIV.2404.01475>.

Keywords: Machine Learning, LLM, Benchmark



Kevin Jablonka leads an independent research group at the Helmholtz Institute for Polymers in Energy Applications of the University of Jena and the Helmholtz Center Berlin where we focusses on designing materials that work in the real world using data-driven techniques. He belongs to a new generation of scientists with a broad skill set, combining expertise in chemistry, materials science, and artificial intelligence. Recently, Kevin has been at the forefront of applying Large Language Models to chemistry and materials science.

Machine Learning for Extreme Climate Event Prediction

C. Herbert^{*}, A. Lovo, V. Mascolo, A. Lancelin, F. Bouchet

^{*} Corresponding author

Laboratoire de Physique, CNRS, ENS de Lyon, France

Extreme climate events such as heat waves, cold spells, extreme precipitation, etc, have major impacts in terms of financial cost, damage to buildings, and human lives. This impact is only expected to grow in a warming climate. Improved prediction capabilities on extended time scales (e.g. from a few days to a few weeks in advance) would therefore be of direct socio-economic values. At the same time, prediction capabilities is tightly linked with fundamental understanding of these events.

Over the past few years, the fast growing use of machine learning methods has opened new prospects for this type of prediction problem. In this talk, I will address some difficulties these approaches meet for rare events, in particular the lack of data to train neural networks, and the need for interpretability of the predictions. I will introduce a simple statistical model based on a joint Gaussian assumption, which outperforms a Convolutional Neural Network for heat wave prediction when data is scarce, and remains competitive for the largest datasets available. By construction, this method leads to interpretable predictions, which I will compare to *a posteriori* interpretation of more complex architectures, such as the CNN and a Scattering Network, still in the case of heat waves.

Keywords: rare event prediction, interpretability, convolutional neural network, scattering network

List of Abstracts – Talks

On the classification of ¹H NMR plants spectra (at an industrial scale) with a combined machine learning and metabolomic approach

Fabien TORRALBA^{12*}; Guillaume HOFFMANN¹; Asma BOURAFAI-AZIEZ²; Christophe MORELL¹

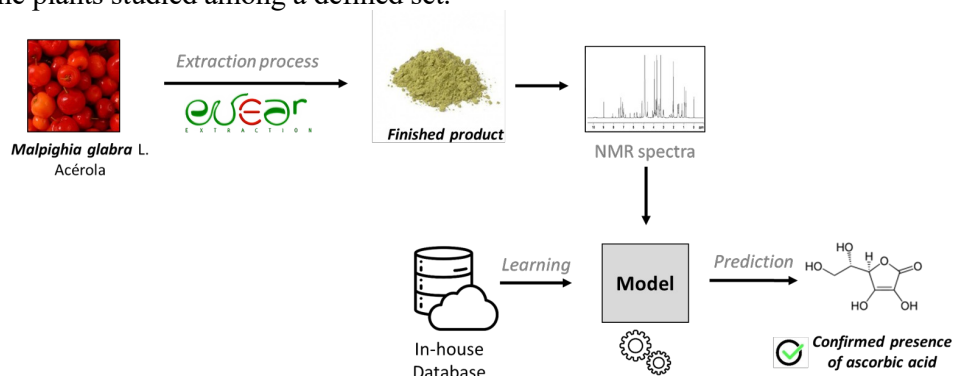
* Corresponding author

¹Université de Lyon, Institut des Sciences Analytiques, UMR 5280, CNRS, Université Lyon 1 - 5, rue de la Doua, F-69100 Villeurbanne, France

²Evear Extraction, 48 Route de Gennes, LD Félines, CEDEX 4, F-49320 Coutures, France

* f.torralba@evear-extraction.com

This presentation will include the results obtained during an ongoing research project of my PhD thesis (in partnership with University of Lyon, France and an industrial partner, EVEAR extraction), on the modeling and intelligent classification of NMR spectroscopic data, using NMR spectra and AI models trained on 4 Nvidia L4 GPUs. The main goal is to develop a classification of plants extract from their NMR spectra database (4000 spectra), aiming to specifically identify the plants studied among a defined set.



This methodology relies on detecting the unique characteristics present in each spectrum, allowing for accurate recognition of the molecules comprising the sample. First a similarity study I presented, from this, early results on a machine learning workflow based on a random forest (RF) algorithm have been obtained. On a side note, a comparison with several other machine learning models will be presented, mainly Support Vector Machines (SVM) and Decision Tree, where some algorithms enhance the results and provide further good predictions. This project promises to significantly improve the speed and accuracy of chemical compound identification on key industrial steps, offering potential applications in various scientific and industrial fields. It represents a notable advancement in the use of NMR spectroscopy, opening new perspectives for the exploration of spectroscopic data in research and beyond.

Keywords: Classification, ¹H NMR, Random Forest, Support Vector Machines, Decision Tree.

NOTE: First Author should be the presenting author.

Analyzing scanning tables data using neural networks

J. Dudouet,^{1*} M. Abushawish,¹ G. Baulieu,¹ O. Stézowski¹

¹Universite Claude Bernard Lyon 1, CNRS/IN2P3, IP2I Lyon, UMR 5822, Villeurbanne, F-69100, France
j.dudouet@ip2i.in2p3.fr

In-beam gamma-ray spectroscopy requires precise Doppler correction. The Advanced GAMMA Tracking Array (AGATA) represents a major development, enabling gamma-ray tracking within the detector. This results in exceptional position resolution and optimal Doppler corrections. AGATA's design features high-purity germanium crystals, each divided into 36 segments to enhance detection accuracy. Position resolution relies on the Pulse Shape Analysis (PSA) algorithm, which identifies interaction points by matching observed signals with a database. Traditionally, this database is built from simulated signals, but employing experimental data promises greater accuracy and robustness. Experimental signals are acquired by scanning crystals with collimated gamma-ray sources using the Strasbourg Scanning Table. Horizontal and vertical scans are performed, and signals are assigned a 3D position via the Pulse Shape Coincidence Scan (PSCS) algorithm. However, PSCS analysis is time-consuming. To address this, a new method based on Long Short-Term Memory (LSTM) networks has been developed. The model incorporates a custom loss function adapted to the scanning setup. Processing time is reduced from five days to one hour. Evaluation against PSCS references demonstrates improved consistency, efficiency, and accuracy.

Keywords: AGATA, Gamma-ray spectroscopy, Digital signal processing, LSTM neural networks

Street-Scale Urban Air Temperature Prediction Using Citizen Weather Stations for Informed Urban Planning.

U. Martinez^{*}; T. Houget; C. V. Nguyen; E. Dellandrea; P. Salizzoni

Ecole Centrale de Lyon, LMFA UMR5509, 69130, Ecully, France

ugo.martinez@ens-lyon.fr

Abstract: Global warming has led to more frequent and intense heat waves worldwide. This phenomenon is particularly severe in cities where the Urban Heat Island effect already elevates temperatures above surrounding rural areas due to heat-absorbing materials and reduced vegetation. These elevated urban temperatures increase mortality rates and strain healthcare systems during extreme heat events. Our research aims then to obtain accurate high-resolution temperature maps using citizen-owned Netatmo weather station networks in Lyon and Turin, for evidence-based urban planning and thermal mitigation strategies. We address the inherent quality control challenges of crowdsourced environmental data through a robust data cleaning framework that identifies and filters unreliable measurements. We evaluate the predictive performance of multiple machine learning approaches (Multiple Linear Regression, Random Forests, Support Vector Regression, and Convolutional Neural Networks). Models are trained using a comprehensive feature set including urban morphology indicators and environmental variables. This work both advances methodological approaches to citizen science data and demonstrates the potential of crowdsourced environmental monitoring for enhancing our understanding of urban microclimates.

Keywords: Urban microclimate, Urban planning, Air temperature mapping, Machine learning.

Quantifying the Electrophilicity of Carbenes by Linking Solid-State Nuclear Magnetic Resonance and Computational Descriptors

Quentin Pessemeesse,*¹ Marie-Ève Perrin,¹ Pierre-Adrien Payard,² Rodolphe Jazzar³

¹ Université Claude Bernard Lyon I, CNRS, CPE-Lyon, UMR 5246, ICBMS, 1 rue Victor Grignard, F-69622 Villeurbanne Cedex, France

² Dunia Innovations, Magnusstraße 11, 12489 Berlin, Germany

³ UCSD-CNRS Joint Research Laboratory (IRL 3555), Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA 92093, United States
quentin.pessemeesse@univ-lyon1.fr

Carbenes are an important class of ancillary ligands for metal catalysts. They possess a lone pair at a carbon atom, which confers nucleophilic, electron-donating properties, as well as a vacant *p* orbital which confers electrophilic, electron-accepting properties. The spectroscopic determination of the electrophilicity of carbenes is important for ligand design. A ⁷⁷Se nuclear magnetic resonance (NMR) scale has been developed, which consists in measuring the chemical shift of carbene-selenium adducts in solution.¹ However, other “parasitic” factors such as steric hindrance influence the ⁷⁷Se chemical shift, limiting the efficiency of the scale.² Solid-state NMR (ss-NMR) suitably probes electrophilicity contributions to the chemical shift by probing orbitals,³ that are least affected by the “parasitic” factors.

A gradient-boosted decision tree approach was used to identify correlations between computed ss-⁷⁷Se chemical shift and computational electrophilicity descriptors. Suitable descriptors were identified, applicable to a wide range of carbene ligands relevant to applications in catalysis, paving the way for spectroscopic determination of carbene electrophilicity.

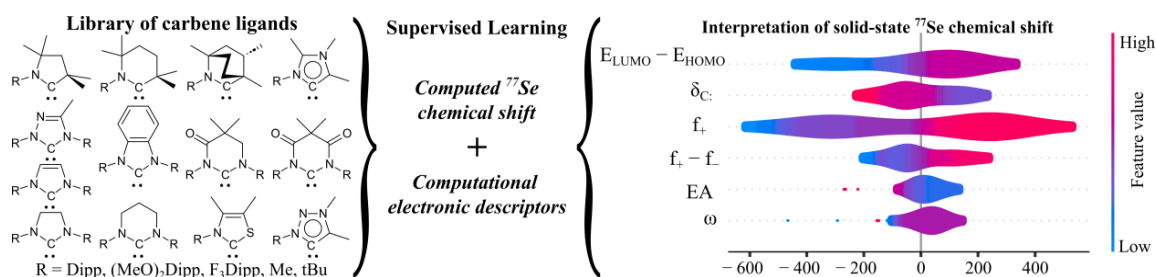


Figure – Methodology to elucidate the link between ⁷⁷Se chemical shift and electrophilicity

References:

- [1] Liske, A.; Verlinden, K.; Buhl, H.; Schaper, K.; Ganter, C. *Organometallics*, **2013**, 32, 5269–5272. [10.1021/om400858y](https://doi.org/10.1021/om400858y) [2] Junor, G. P.; Lorkowski, J.; Weinstein, C. M.; Jazzar, R.; Pietraszuk, C.; Bertrand, G. *Angew. Chem. Int. Ed.*, **2020**, 59, 22028–22033. [10.1002/anie.202010744](https://doi.org/10.1002/anie.202010744) [3] Engl, P. S.; Santiago, C. B.; Gordon, C. P.; Liao, W.-C.; Fedorov, A.; Copéret, C.; Sigman, M. S.; Togni, A. *J. Am. Chem. Soc.*, **2017**, 139, 13117–13125. [10.1021/jacs.7b06947](https://doi.org/10.1021/jacs.7b06947)

Keywords: Nuclear Magnetic Resonance (NMR), Spectroscopy, Ligands, Carbenes, Descriptors

Electrostatically Embedded QM/MM Study of the Potential-Dependent Reorientation of Pyridine on Au(111)

M. Gu; C. Michel, S. N. Steinmann*

ENS de Lyon, CNRS, LCH, UMR 5182, 69342, Lyon cedex 07, France

stephan.steinmann@ens-lyon.fr

Electrified interfaces are the key to heterogeneous electrocatalysis. To achieve an atomistic description of the reactivity, grand-canonical density functional theory (GC-DFT) is one of the most popular and convenient approaches. However, the accuracy of the widely used implicit solvation models, that are usually used in combination with GC-DFT, is questionable. We have developed a quantum mechanics (QM)/molecular mechanics (MM) approach, applied to surfaces and solvent, respectively, to model the solvent in a more realistic way without significantly increasing the computational cost.¹ In this work, the hybrid QM/MM scheme with electrostatic embedding is applied to a system where the water solvent interacts with moderate strength with the metallic gold electrode: the potential-dependent reorientation of pyridine adsorbed on Au(111), which is experimentally well characterized. Three coordination modes of pyridine to Au surface have been reported: parallel adsorption of the aromatic ring, tilted and perpendicular adsorption via lone-pair electrons of the N atom.² For each mode, the grand-canonical adsorption energy has been evaluated as a function of potential and coverage to determine the most favorable one as a function of the potential. In contrast to implicit solvents³, the transition potential is predicted in reasonable agreement with experiment, see Figure 1.

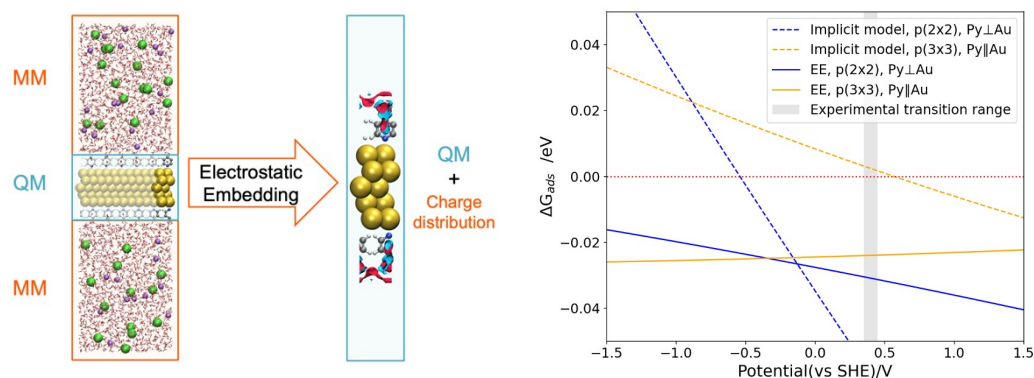


Figure 1 – Left: Schematic picture of our QM/MM scheme. Right: Adsorption energy per Au surface atom as function of electrochemical potential. The transition potential obtained by EE (-0.4 V vs SHE) is more consistent than when using an implicit solvent (-0.9 V) compared to the experimental results of ref [2] (0.4 V).

Keywords: grand-canonical DFT, electrified interfaces, QM/MM, solvation

Reference

- (1) Abidi, N.; Steinmann, S. N. An Electrostatically Embedded QM/MM Scheme for Electrified Interfaces. *ACS Appl. Mater. Interfaces* **2023**, *15* (20), 25009–25017.
- (2) Cai, W.-B.; Wan, L.-J.; Noda, H.; Hibino, Y.; Ataka, K.; Osawa, M. Orientational Phase Transition in a Pyridine Adlayer on Gold(111) in Aqueous Solution Studied by in Situ Infrared Spectroscopy and Scanning Tunneling Microscopy. *Langmuir* **1998**, *14* (24), 6992–6998.
- (3) Steinmann, S. N.; Sautet, P. Assessing a First-Principles Model of an Electrochemical Interface by Comparison with Experiment. *J. Phys. Chem. C* **2016**, *120* (10), 5619–5623.

Towards smart growth of functional oxides with on-demand properties?

R. Bachelet*, C. Furgeaud, M. Bounab, T. Zhu, C. Botella, P. Regreny, R. Rousseau, G. Saint-Girons

CNRS, Ecole Centrale de Lyon, INSA Lyon, Université Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69130 Ecully, France

* romain.bachelet@ec-lyon.fr

The “*Functional Materials and Nanostructures*” team at INL is closely interested in the use of deep learning in these research areas. The team possesses unique expertise in the growth of functional oxides by molecular beam epitaxy (MBE), a versatile elaboration tool to grow various oxide heterostructures (solid-solutions, superlattices, phases, heterogeneous interfaces,...) with diversified functional properties (thermoelectric, hyperbolic, optoelectronic,...) [1-2]. The team is currently developing an *operando* control of the growth through unique and innovative couplings of *in-situ* and *real-time* measurements during oxide growth (curvature measurement, ellipsometry, RHEED, flux monitoring,...) (Figure). Beyond the concept and experimental preliminary results, the interest in machine learning comes into play for the two following main objectives: 1/ screening new materials with novel properties and breaking with the state of the art, and 2/ smart oxide growth through self-regulation of epitaxy reactor.

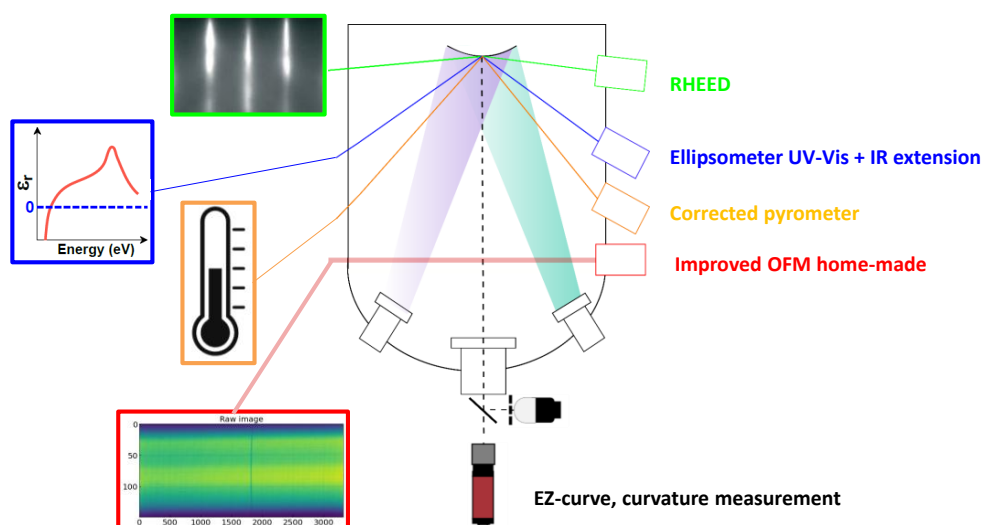


Figure: sketch of the smart growth, from various *operando* measurements of the structural and physical properties.

References

- [1] D. Han *et al.*, ACS Appl. Electron. Mater. **3**, 3461 (2021); <https://doi.org/10.1021/acsaelm.1c00425>
- [2] M. Bouras *et al.*, ACS Photonics **6**, 1755 (2019); <https://doi.org/10.1021/acsp Photonics.9b00485>

Keywords: Epitaxy, functional oxides, operando measurements, deep learning, smart growth

Synthesis of Boron-rich B_xC Thin film via Chemical Vapor Deposition

A. O. Afolabi*; C. Marichy; C. Journet; C. Bousige.

Laboratory of Multimaterials and Interfaces, Claude Bernard University Lyon 1, UMR CNRS 5615. Chevreul Building, 6 rue Victor Grignard, 69622 Villeurbanne, France.

abdulhamid.afolabi@univ-lyon1.fr

Boron-carbon (B_xC) materials are wide band gap semiconductors, and the band gap has been reported to correlate with its composition, enabling diverse applications. This study focuses on chemical vapor deposition (CVD) of boron rich B_xC films from Triethylborane (TEB) with the aim to model the boron to carbon (B/C) ratio.

The CVD process parameters include TEB flux, deposition temperature, time, carrier gas flux (H_2 and Ar), and cooling gas flux. Given the numerous possible parameter combinations, we are employing a two-step optimization approach. First, we use a design of experiment step to screen the CVD parameters and define a design space. The collected experimental data then serve as the initial dataset for the next step of Bayesian optimization with the objective function of maximizing the B/C ratio, utilizing Gaussian Process and Random Forest Regressors as surrogate models. The algorithm iteratively suggests the next experiment to carry out by data-driven recommendations, hence reducing the number of required experiments. The final model then enables predictive tuning of the B/C ratio.

So far, we have identified temperature and TEB flux as the most relevant parameters to model the B/C ratio. Future work would focus on further optimization of the parameters and evaluating the performance of the models.

Keywords: Chemical vapor deposition, Boron-carbon materials, Design of Experiment, Bayesian optimization, Machine learning in materials science.

Use of foundation model for defects in BCC metals

P. Grigorev^{1*}, T. D. Swinburne², J. R. Kermode³

* Corresponding author

¹CNRS, INSA Lyon, Université Claude Bernard Lyon 1, MATEIS, UMR5510, 69621
Villeurbanne, France

²Aix-Marseille Université, CNRS, CINaM UMR 7325, Campus de Luminy, 13288
Marseille, France

³Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick,
Coventry CV4 7AL, United Kingdom

E-mail of corresponding author Petr.Grigorev@cnrs.fr

Recent advancement of machine learning force fields allowed the development of universal models capable of describing large number of elements and chemical environments. Here we test a novel model MACE-MP0 which is based on MACE architecture and is trained on a public database of 150k inorganic structure types (1.5M configurations in total) composed of 89 elements. We look at properties of point and extended defects in three BCC metals: W, Mo, Nb. For the case of W we demonstrate how the model can be used as a “foundation model” allowing for further fine tuning for a given application.

Keywords: Machine learning interatomic potentials, foundation model, finetuning, atomistic simulation

List of Participants

Benjamin ABECASSIS	benjamin.abecassis@ens-lyon.fr
Pavel AFANASIEV	pavel.afanasiev@ircelyon.univ-lyon1.fr
Abdulhamid AFOLABI	abdulhamid.afolabi@univ-lyon1.fr
Tristan ALBARET	tristan.albaret@univ-lyon1.fr>
Kevin ALHADA-LAHBABI	kevin.alhada-lahbabi@insa-lyon.fr
Abdulrahman ALLOUCHE	allouche@univ-lyon1.fr
Cesar ALVAREZ LLAMAS	cesar.alvarez-llamas@univ-lyon1.fr
Abderrahmane AMGOUNE	abderrahmane.amgoune@univ-lyon1.fr
David AMRAM	d.amram@ip2i.in2p3.fr
Olivier AROULE	olivier.aroule@isa-lyon.fr
Romain BACHELET	romain.bachelet@ec-lyon.fr
Francesco BANFI	francesco.banfi@univ-lyon1.fr
Guillaume BAULIEU	g.baulieu@ip2i.in2p3.fr
Jörg BEHLER	joerg.behler@ruhr-uni-bochum.de
Ismail BEN YOUSSEF	ismail.ben-youssef@insa-lyon.fr
Julien BERNARD	julien.bernard@insa-lyon.fr
Auday BERRO	auday.berro@univ-lyon1.fr
Michaël BEUVE	michael.beuve@univ-lyon1.fr
Kévin BILAI BILOA	kevin-gabriel.bilai-bilola@univ-lyon1.fr
Dylan BISSUEL	dylan.bissuel@univ-lyon1.fr
Florian BLANC	florian.blanc@isa-lyon.fr
Latifa BOUCHET	latifa.bouchet@univ-lyon1.fr
Alexis BOUDON	a.boudon@ip2i.in2p3.fr
Joanne BOULOS	j.boulos@groupeginger.com
Colin BOUSIGE	colin.bousige@univ-lyon1.fr
Mathieu CANCADE	mathieu.cancade@ens-lyon.fr
Ruben CHECA	ruben.checa@ircelyon.univ-lyon1.fr
Henry CHERMETTE	henry.chermette@univ-lyon1.fr
Francisco CHINESTA	Francisco.Chinesta@ensam.eu
Olivier COCHET-ESCARTIN	olivier.cochet-escartin@univ-lyon1.fr
Yannick COPIN	y.copin@ipnl.in2p3.fr
Yohann DE CASTRO	yohann.de-castro@ec-lyon.fr
Matheus DE OLIVEIRA BISPO	matheus.de-oliveira-bispo@univ-amu.fr
Roland DENIS	denis@math.univ-lyon1.fr
Hatem DIAF	hatem.diaf@univ-lyon1.fr
Jan DIEKMANN	jan.diekmann@uni-muenster.de
Jérémie DUDOUET	j.dudouet@ip2i.in2p3.fr
Jérôme DUPUY	jerome.dupuy@insa-lyon.fr
Eric EHRET	eric.ehret@ircelyon.univ-lyon1.fr
Fabienne FACHE	fabienne.fache@univ-lyon1.fr
Latifa FAKRI-BOUCHET	latifa.bouchet@univ-lyon1.fr
Sofiane FERCHICHI	sofiane.ferchichi@ifpen.fr
Gabriel FERRO	gabriel.ferro@univ-lyon1.fr
Elise FOURNIER	elise.fournier@cpe.fr
Li FU	li.fu@ec-lyon.fr
Ludovic GARDRÉ	ludovic.gardre@univ-lyon1.fr

Aurélien GARIVIER	aurelien.garivier@ens-lyon.fr
Petr GRIGOREV	petr.grigorev@cnrs.fr
Mingjun GU	mingjun.gu@ens-lyon.fr
Céline GUILLEMAIN	celine.guillemain@inrae.fr
Isa HELAL	isa.helal@ec-lyon.fr
Matthias HILLENKAMP	matthias.hillenkamp@univ-lyon1.fr
Corentin HERBERT	corentin.herbert@ens-lyon.fr
Guillaume HOFFMANN	guillaume.hoffmann@univ-lyon1.fr>
Heigo ERS	heigo.ers@ens-lyon.fr
Adamu aminu IDRIS	adamu-aminu.idris@univ-lyon1.fr
Kevin JABLONKA	mail@kjablonka.com
Gauthier JACQUIN	gauthier.jacquin@phelma.grenoble-inp.fr
Steve JATIERE	steve.jatiere@univ-lyon1.fr
Inyoung JUNG	inyoung.jung@univ-lyon1.fr
Ibrahim KHALIL	ibrahim.khalil@ircelyon.univ-lyon1.fr
Teodoro LAINO	TEO@zurich.ibm.com
Inès LANDA	ines.landa@etu.umontpellier.fr
Yu LI	yu.li@ens-lyon.fr
Hugo LILTI	hugo.lilti@ircelyon.univ-lyon1.fr
Fangbing LIU	fangbing.liu@univ-lyon1.fr
Claire LOISON	claire.loison@univ-lyon1.fr
Aurore LOISY	aurore.LOISY@univ-amu.fr
Nazila MAHMOUDI	mahmoudi@in2p3.fr
Mathieu MAILLARD	mathieu.maillard@univ-lyon1.fr
Jean-charles MAJESTÉ	majeste@univ-st-etienne.fr
Benoît MARTELAT	benoit.martelat@cpe.fr
Ugo MARTINEZ	ugo.martinez@ens-lyon.fr
David MARTIN-CALLE	david.martin-calle@univ-lyon1.fr
Matthieu MASSON	matthieu.masson@inrae.fr
Laetitia MATIGNON	laetitia.matignon@univ-lyon1.fr
Micaïs MENEAU	micaïs.meneau@univ-lyon1.fr
Cécile MIÈGE	cecile.miege@inrae.fr
Pierre MIGNON	pierre.mignon@univ-lyon1.fr
Virginie MONNIER	virginie.monnier@ec-lyon.fr
Damien MONTARNAL	damien.montarnal@univ-lyon1.fr
Franck MORFIN	franck.morfin@ircelyon.univ-lyon1.fr
Patrick NEDELEC	patrick.nedelec@univ-lyon1.fr
Lana NEORICIC MACLOT	lana.neoricic-maclot@univ-lyon1.fr
Clément NOËL	clement.noel@univ-lyon1.fr
Olha KRYVA	olha.kryva@etu.ec-lyon.fr
Stéphane PAILHÈS	stephane.pailhes@univ-lyon1.fr
Jean-luc PAROUTY	Jean-Luc.Parouty@simap.grenoble-inp.fr
Théo PESENTI	theo.pesenti@univ-lyon1.fr
Quentin PESSEMESE	quentin.pessemesse@univ-lyon1.fr
Olivier PIERRE-LOUIS	olivier.pierre-louis@univ-lyon1.fr
Guy RAFFIN	Guy.RAFFIN@isa-lyon.fr
Jean RAYNAUD	jean.raynaud@cnrs.fr
Benedetta RIGATELLI	benedetta.rigatelli@univ-lyon1.fr
Steven ROLDAN GOMEZ	steven.roldan-gomez@univ-lyon1.fr

Vincent MOTTO-ROS	vincent.motto-ros@univ-lyon1.fr
David ROUSSEAU	david.rousseau@univ-angers.fr
Roman ROUSSEAU	roman.rousseau@ec-lyon.fr
victor SABANZA GIL	victor.sabanzagil@epfl.ch
Chloé SANZ	chloe.sanz@univ-lyon1.fr
Léo SCHNEIDER	leo.schneider@univ-lyon1.fr
Mohammed el amine SEHABA	mea.sehaba@univ-lyon2.fr
Gyeongseob SONG	gyeongseob.song@ec-lyon.fr
Olivier STEZOWSKI	stezow@ipnl.in2p3.fr
Pierre STRAZEWSKI	strazewski@univ-lyon1.fr
Rocco SUANNO	rocco.suanno@univ-lyon1.fr
Matthieu THOMEER	matthieu.thomeer@etu.univ-lyon1.fr
Théodore TILLEMENT	t.tillement@minerals-and-ai.com
Josene TOLDO	Josene.toldo@univ-lyon1.fr
Fabien TORRALBA	f.torralba@eveal-extraction.com
Gaël TRAN	gael.tran@univ-lyon1.fr
Adam TRIGUI	a.trigui@ip2i.in2p3.fr
William VAGINAY	w.vaginay@ip2i.in2p3.fr
Anu VASHISHTHA	anu.vashishtha@univ-lyon1.fr
Christian VEROLLET	c.verollet@ip2i.in2p3.fr
Sebastien VIRET	s.viret@ip2i.in2p3.fr
christophe YBERT	christophe.ybert@univ-lyon1.fr
Marie-line ZANOTA	marie-line.zanota@cpe.fr