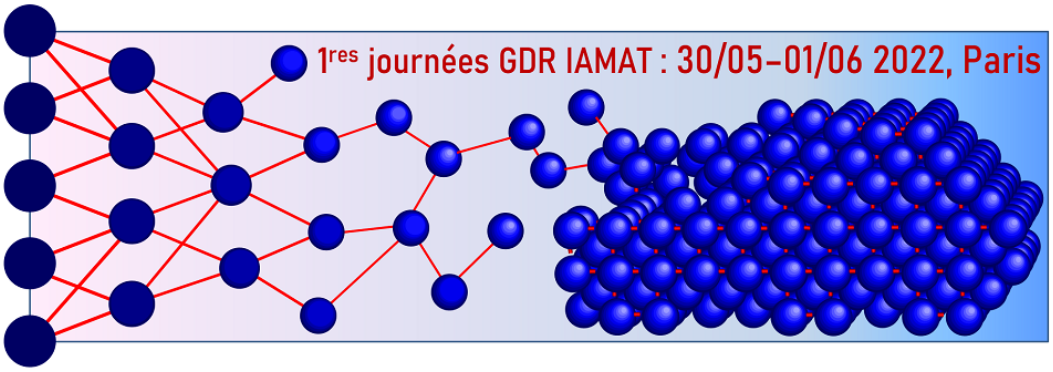
Liste des Contributions

GDR IAMAT

30 mai - 1 juin 2022, Sorbonne université, Paris



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version 30/05-v3

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lundi 30 mai					mardi 31 mai								mercredi 1 juin				
					10 mm	9:00	9:10	**A**	**Introduction : Florent Calvo (CNRS, INP)**								
					50 mm	9:10	10:00	**A**	**Invité: Maxime Sangnier**				*50 mm*	9:00	9:50	**25**	**Invité: Gérard Ramstein**
					50 mm	10:00	10:50	**A**	**Invité: Jean-Luc Parouty**				*15 mm*	9:50	10:05	25	Plénière: Charpentier
					30 mm	10:50	11:20	**E**	Pause café				*15 mm*	10:05	10:20	25	Plénière: Percebois
					15 mm	11:20	11:35	**106/108**	Parallèle: Karcz / Forster				*15 mm*	10:20	10:35	25	Pause café
					15 mm	11:35	11:50	**106/108**	Parallèle: Maillard / Monchot				*15 mm*	10:35	10:50	25	Plénière: Sohier
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					80 mm	12:35	14:00	**E**	Déjeuner								
					50 mm	14:00	14:50	**A**	**Invité: Gian-Marco Rignanese**								
					50 mm	14:50	15:40	**A**	**Invité: Sandrine Lyonnard**								
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					30 mm	15:55	16:25	**E**	Pause café								
					15 mm	16:25	16:40	**106/108**	Parallèle: Almeida de Mendonca / Allera								
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					15 mm	16:55	17:10	**106/108**	Parallèle: Meier / Rateau								
					15 mm	17:10	17:25	**106/108**	Parallèle: Swinburne / Garel								
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					90 mm	17:40	19:10	**P**	Posters								
	9:00	- 10:30	**A**	Accueil - Enregistrement													
15 mm	10:30	- 10:45	**A**	Café d'accueil													
30 min	10:45	- 11:15	**A**	**Marco Saitta, Benoît Devincre (CNRS), Introduction: Gérard Biau**													
30 min	11:15	- 11:45	**A**														
15 mm	11:45	- 12:00	**A**	**François Willaime: DIADEME**													
90 mm	12:00	- 13:30	**P**	Déjeuner													
50 mm	13:30	- 14:20	**A**	**Invité: Cosmin Marinica**													
50 mm	14:20	- 15:10	**A**	**Invité: Vincent Favre-Nicolin**													
50 mm	15:10	- 16:00	**A**	**Invité: Nicola Marzari**													
30 mm	16:00	- 16:30	**A**	Pause café													
50 mm	16:30	- 17:20	**A**	Flash labo (10)													
50 mm	17:20	- 18:10	**A**	Flash labo (10)													
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Salles
A = Auditorium
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108 = Tour 44 salle 108
E = espace lunch Tour 44
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2 Présentations invités

Lundi 30 mai

11h15 : Gérald Biau (directeur SCAI) : *introduction générale*

13h30 : Cosmin Marinica (CEA) : *(Physics informed) Machine Learning for atomistic materials Science*

14h20 : Vincent Favre-Nicolin (ESRF) : *AI for automated data collection and analysis-an ESRF perspective*

15h10 : Nicola Marzari (EPFL) : *Digital infrastructure empowering materials discovery*

Mardi 31 mai

9h10 : Maxime Sangnier (Sorbonne université) : *Un panorama des méthodes de classification et clustering*

10h00 : Jean-Luc Parouty (SIMAP) : *Deep Learning, histoire et principes, de la régression aux GANs*

14h00 : Gian-Marco Rignanese (UC Louvain) : *OPTIMADE : A Common REST API for Materials Databases Interoperability*

14h50 : Sandrine Lyonnard (SyMMES) : *Accelerating the characterization of batteries : multimodal and multitechniques integrated workflows*

Mercredi 1 juin

9h00 : Gérard Ramstein (université Nantes) : *Solving optimization problems with machine learning - Application to materials science*

3 Présentations des Laboratoires

1. Apport du machine learning à la modélisation à l'échelle atomique des oxydes d'actinides
   Messina Luca <Luca.MESSINA@cea.fr> (CEA, DES, IRESNE, DEC)

2. Artificial Intelligence at the IPCMS
   Weinmann Dietmar <dietmar.weinmann@ipcms.unistra.fr> (IPCMS, Strasbourg)

3. Consortium : LAAS-CNRS (Toulouse, France), CEA-DAM (Arpajon, France), CNR-IOM (Trieste, Italie)
   Hémeryck Anne <anne.hemeryck@laas.fr> (LAAS, Toulouse)

4. Développement de Machine Learning Potential pour les Matériaux Hybrides Poreux
   Dupuis Romain <rdupuisbelin@gmail.com> (Institut Européen des membranes, ICGM, Montpellier)

5. Développement et utilisation du Machine learning au laboratoire LMCE
   Bottin Francois <francois.bottin@cea.fr> (CEA, DAM, DIF)

6. DIADEME / FAST NANO : High throughput characterization & synthesis of nanomaterials assisted by machine learning
   Taché Olivier <olivier.tache@cea.fr> (NIMBE, Nanometric Organisation Laboratory)

7. Energy landscapes from Bayesian and machine-learning methods
   Trassinelli Martino <Martino.Trassinelli@insp.jussieu.fr> (Institut des NanoSciences de Paris, Sorbonne Université-CNRS)

8. Geosciences Environment Toulouse : Materials research in Earth Sciences, and Christmas list
   Méheut Merlin <merlin.meheut@get.omp.eu> (Géosciences Environnement Toulouse, 2 - Géochimie des Isotopes Stables (France))

9. High Throughput Experimental Studies of Hard Magnetic Films @ Institut NEEL
   Devillers Thibaut <thibaut.devillers@neel.cnrs.fr>, (Institut NEEL)

10. l'IA appliquée à la microscopie électronique et à la modélisation de la plasticité
    Amara Hakim <hakim.amara@onera.fr> (Laboratoire d'étude des microstructures)

11. Laboratoire Modélisation multi-échelle et suivi de Performance du CEA - LITEN
    Van Roekeghem Ambroise <ambroise.vanroekeghem@cea.fr> (CEA-Grenoble)

12. Laboratoire SIMAP : activités autour de l'IA
    Deschamps Alexis <alexis.deschamps@grenoble-inp.fr> (SIMAP - Grenoble INP)

13. Machine Learning pour le design de superalliages monocristallins à base de nickel et la modélisation de leur microstructure
    Degeiter Matthieu <matthieu.degeiter@onera.fr> (DMAS, ONERA)

14. Machine-Learning pour l'instrumentation scientifique, la nano-analyse des matériaux, et la simulation au GPM
    Demange Gilles <gilles.demange@univ-rouen.fr> (Groupe de Physique des matériaux)

15. Présentation de l'ICMPE
    Crivello Jean-Claude <crivello@icmpe.cnrs.fr> (ICMPE)

16. Présentation des activités de l'IMPMC en IA & Matériaux
    Saitta Antonino Marco <marco.saitta@sorbonne-universite.fr> (Institut de Minéralogie, de

Physique des Matériaux et de Cosmochimie)

17. Présentation du laboratoire d'Analyse Microstructurale des Matériaux (LA2M) - CEA Saclay
    Lafond Clément <clement.lafond@cea.fr> (Laboratoire d'analyse Microstructurale des Matériaux)

18. IA and Machine Learning at CEMES, Toulouse
    Benoit Magali <magali.benoit@cemes.fr> (CEMES-CNRS)

19. Institut des Matériaux de Nantes Jean Rouxel
    Braems Isabelle <isabelle.braems@cnrs-imn.fr> (IMN-CNRS)

20. Equipe Modélisation Moléculaire impliquée en catalyse hétérogène
    Corral Valero Manuel <manuel.corral-valero@ifpen.fr> (IFPEN)

21. Institut de Chimie de la Matière Condensée de Bordeaux
    Lecoutre Carole <carole.lecoutre@icmcb.cnrs.fr> (ICMCB-CNRS)

22. French Collaborating Research Group at ESRF, Grenoble
    Micha Jean-Sébastien <micha@esrf.fr> (ESRF)

23. UMET : Unité Matériaux et Transformations
    Rolland Manon <manon.rolland@univ-lille.fr> (Université de Lille)

24. Transformations of matter involved in processes for bulk ceramics and surface treatment
    Fabrice Rossignol <fabrice.rossignol@unilim.fr> (Institute of Research for Ceramics)

25. The CEA Grenoble, IRIG, MEM laboratory
    Joel Eymery <joel.eymery@cea.fr> (CEA Grenoble, IRIG, MEM)

26. Graph Theory for Molecular Dynamics Simulations
    Marie-Pierre Gaigeot <mgaigeot@univ-evry.fr> (LAMBE, université Evry)

4 Résumé des présentations orales

(Physics informed) Machine Learning for Atomistic Materials Science

Alexandra Goryaeva , Clovis Lapointe , Jacopo Baima , Allera Arnaud , Thomas Bilyk , Thomas Swinburne , and Mihai-Cosmin Marinica*[1]

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Résumé

We will present recent advances in atomistic material simulations by means of machine learning and data-driven approaches. In order to provide reliable results in the field of physics, Machine Learning must be trained on logically coherent data provided by well established methods from the community of physics. If trained on physical data, it can be of great help when the traditional approaches are limited and/or their direct application is hindered by factors such as high computational cost. In addition, multi-scale approaches in materials science face a traditional dichotomy in the choice of the atomistic force fields: robust, accurate and numerically expensive ab initio methods against less transferable but fast empirical methods. The ML methods propose a third avenue that allows control of the balance between the accuracy and numerical efficiency. Moreover, the ML-based vision of fundamental concepts in materials science, such as structural defects, can augment and revise traditional interpretations.

In previous years, we have used ML to advance the knowledge of materials related to energy applications. Using the recently developed package MiLaDy (Machine Learning Dynamics) (2): (i) we redefine the concept of defects in materials science (1,3); (ii) we provide reliable force fields for complex defects such as interstitial, dislocation loops, dislocations; (iii) we are able to explore the atomistic free energy landscape (including migration energies (nn, mm)) of point defects in metals with ab initio accuracy up to the melting temperature (4), and, finally, (iv) we are able to propose surrogate models that bypass the traditional approaches (5). We exemplify and discuss in the framework of experimental findings the case of energetic landscape of defects in body centered and face centered cubic metals..

(1) K. Arakawa , M.-C. Marinica et al. Nature Mat. 19, 508(2020) ; R. Alexander et al. Phys. Rev. B 94, 024103 (2016)

(2) M.-C. Marinica, A. M. Goryaeva, T. D. Swinburne et al, MiLaDy - Machine Learning Dynamics, CEA Saclay, 2015-2021 ; A.M. Goryaeva, J.-B. Maillet, M.-C. Marinica. Comp. Mater. Sci. 166, 200 (2019)

(3) A. M. Goryaeva et al. Nature Commun. 11, 4691 (2020)

(4) C. Lapointe et al. (to be submitted). , T.D. Swinburne, M.-C. Marinica, Phys. Rev.

*Intervenant

Machine-learning aided calculation of atomic-scale properties in chemically disordered (U, Pu)O2 fuels

Maciej Karcz*[1], Serenah Rajaonson[1], Didier Bathellier[1], Luca Messina[1], Eiji Kawasaki[2], Maylise Nastar[3], Thomas Schuler[3], and Emeric Bourasseau[1]

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[2]Université Paris-Saclay – CEA, List, F-91120, Palaiseau France – France
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Résumé

Machine-learning methods are nowadays of common use in scientific research to augment the predictability of physical models. For example, they can aid in optimizing the physicochemical properties of new materials, or help in the characterization of highly complex chemical compounds. An especially challenging problem arises in the modeling of chemically disordered solid solutions, for which some properties depend on the distribution of chemical species in the crystal lattice - the number of possible configurations is so high that the use of conventional atomic-scale methods is challenging. An example of such compound is uranium-plutonium mixed oxides. In this work, we rely on deep generative modelling to optimize the exploration of the configuration space and estimate the physical properties of (U,Pu)O2, namely the concentration of thermal defects. This is an important property needed to model the microstructure evolution of this kind of fuel. A mixture density network is trained on a limited amount of data to predict the probability distribution of the formation energy of a defect Ef , that can be applied for the computation of thermal equilibrium concentration of defects. This approach can be also used for other properties that depend on local atomic configurations, such as formation entropies, migration energies, or attempt frequencies. Furthermore, this method can be relevant for other disordered materials such as high-entropy alloys.

*Intervenant

NESTED_FIT : DEVELOPMENTS AND TESTS

Lune Maillard*[1], Martino Trassinelli[1], and Fabio Finocchi[2]

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Résumé

Nested Sampling is a sampling method that is used to characterise multidimensional functions. On the one hand, it can be used to calculate the Bayesian evidence and thus assign probabilities to different models from a same set of data. On the other hand, it can be used to evaluate the partition function of energy landscapes. The Nested Sampling algorithm's benefit consists on turning the multi-dimensional integral into a one dimensional integral by a dynamically evolving sampling (live points), thus considerably reducing the computational needs. A major bottleneck of this algorithm lies on finding new sampling points, expecially when several maxima (resp. minima) are present. The recognition via machine learning methods of cluster structures of the live points, corresponding to the function's maxima (resp. minima), allows to adapt the search of new points more efficiently. In a previous version of the nested_fit code, a new point search based on a random walk and a clustering recognition based on the Mean Shift algorithm were implemented. Here, we aim to present several new methods that have been added to the nested_fit code, both to search for new points and to perform clustering. These methods are tested and compared on a variety of examples including two benchmarks examples for energies: the harmonic potential and the Lennard - Jones clusters.

*Intervenant

Combining machine learning and ab initio enhanced sampling methods for prebiotic chemical reactions

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Résumé

The study of the thermodynamics, kinetics, and microscopic mechanisms of chemical reactions in solution requires the use of advanced free-energy methods for predictions to be quantitative. This task is however a formidable one for atomistic simulation methods, as the cost of quantum-based ab initio approaches, to obtain statistically meaningful samplings of the relevant chemical spaces and networks, becomes exceedingly heavy. In this work, we critically assess the optimal structure and minimal size of an ab initio training set able to lead to accurate free energy profiles sampled with neural network potentials. The results allow to propose an ab initio protocol where the ad hoc inclusion of a machine-learning (ML)-based task can significantly increase the computational efficiency, while keeping the ab initio accuracy and, at the same time, avoiding some of the notorious extrapolation risks in typical atomistic ML approaches. We focus on two representative, and computationally challenging, reaction steps of the classic Strecker-cyanohydrin mechanism for glycine synthesis in water solution, where the main precursors are formaldehyde and hydrogen cyanide. We demonstrate that indistinguishable ab initio-quality results are obtained, thanks to the ML-subprotocol, at about one order of magnitude less of computational load

*Intervenant

Ab initio Canonical Sampling based on Variational Inference

Aloïs Castellano*[1], Francois Bottin[2], Johann Bouchet[3], Antoine Levitt[4,5], and Gabriel Stoltz[4,5]

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Résumé

Finite temperature calculations, based on ab initio molecular dynamics (AIMD) simulations, are a powerful tool able to predict material properties that cannot be deduced from ground state calculations. However, the high computational cost of AIMD limits its applicability for large or complex systems. To circumvent this limitation we introduce a new method named Machine Learning Assisted Canonical Sampling (MLACS), which accelerates the sampling of the Born–Oppenheimer potential surface in the canonical ensemble by iteratively training a Machine Learning Interatomic Potential (MLIP) (1).
The key idea of MLACS is to best reproduce the canonical distribution of atomic positions generated byAIMD simulations by the one induced by the MLIP potential. We prove that this goal can be reached by minimizing the Kullback–Leibler and Fisher divergences (2) for these two distributions and that a non-trivial least-squares (LS) problem is then obtained. The MLIP linear parameters, solutions of the LS problem, are finally computed by using the following self-consistent variational procedure: start with a few atomic configurations, compute their energies, forces and stresses at the ab initio level, check the convergence of specific observables, compute the linear MLIP parameters, build a MLIP potential, perform a molecular dynamic (MD) run using the MLIP and extract new atomic configurations from the trajectory. This SC procedure is repeated until convergence.

*Intervenant

Observing the birth of crystals through machine-learning assisted simulations

Gaétan Laurens[1], Jacek Goniakowski[2], and Julien Lam*[3]

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[2]Institut des Nanosciences de Paris (INSP) – Université Pierre et Marie Curie - Paris 6 – France
[3]Center for Nonlinear Phenomena and Complex Systems – Belgique

Résumé

While crystals in material science are ubiquitous, the mechanisms of their formation which spans from nucleation to crystal growth remain one of the most intriguing process in nature. Better understanding crystallization would allow for a rational control of material engineering and possibly the development of novel functional materials and technological applications. From the fundamental point of view, numerous works have been dedicated to elucidating the emergence of the nucleation core and its role in controlling the final crystal structure. For instance, it is now possible to observe the crystal birth with electron microscopy, and colloidal science has also provided numerous experimental results on nucleation. Yet, while numerical simulations should have been a pivotal instrument to investigate crystallization at the atomistic level, studying nucleation require large scale simulations in order to observe the phase transition. As such, most works based on simulations have only focused on simple model materials thus preventing from targeting specific technological applications.
In this presentation, we will introduce innovative numerical tools based on machine-learning approaches and show how they can be employed to probe the nucleation processes in more complex materials. In particular, we focused on zinc oxide crystallization for which we developed a linear-based machine-learning interaction potential that can surpass all of the current classical models. Then, we combined large scale simulations and data-driven structure analysis to study the crystal nucleation. One key aspect of our work was to demonstrate that predictions of non-classical nucleation that were obtained with model materials including Lennard-Jones and hard spheres systems are still valid. Altogether, our results seems to demonstrate a universality of the crystallization processes ranging from soft to condensed matter.

*Intervenant

Analysis of high-resolution transmission electron microscopy images by deep learning: example of AgCo nanoalloys

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Résumé

To fully exploit the potential of nano-objects for various applications, robust methods of on-demand synthesis are needed. Their development relies on the possibility to characterize samples quickly and quantitatively. Aberration-corrected transmission electron microscopes with the high-resolution technique (HRTEM) allow obtaining images at atomic resolution. However, image analysis can be time-consuming, especially when a statistically significant number of particles must be evaluated if carried out manually. With this contribution, we automate crucial parts of this process for fast and reliable analysis.
Our approach coupling atomistic simulations to deep learning methods is aimed to improve the analysis capabilities of high-resolution electron microscopy. Although deep learning methods have barely been used for the analysis of HRTEM images, we believe that they are perfectly suited for this task, mostly due to the possibility to numerically create large and realistic datasets (1).

In a first step, molecular dynamics simulations based on a second moment tight-binding potential are used to generate a large number of configurations of AgCo bimetallic particles close to equilibrium at room temperature (2). Final snapshots from the simulations are extracted and serve as a basis for the generation of synthetic HRTEM images obtained using the multi-slice technique (3). During this process of image generation, special attention is given to the variability and realism regarding the experimental conditions that we want to address.

Finally, we train several convolution neural networks to explore the possibilities of analysis made possible by this approach (4). Firstly, they can be used to classify images of particles with respect to their chemical ordering (segregated core-shell or Janus bi-compartmented configuration). Secondly, a similar network can be used for regression, allowing to recover properties of the nanoalloy particles (size and composition) from the HRTEM images. Finally, using an auto-encoder network, it is possible to suppress the shot noise due to the

*Intervenant

Deep Learning based particle size estimation: application to agglomerated titanium dioxide particles measured by scanning electron microscopy

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[1]Laboratoire National de Métrologie et dÉssais [Trappes] (LNE) – EPIC – 29 avenue Roger Hennequin 78197 Trappes cedex, France

Résumé

In many cases, the estimation of particle size distribution of a nanoparticle population remains a major challenge for the industrial development of nanomaterials. Titanium dioxide (TiO2) in nanoparticulate form is produced in very large quantities for intensive use in many applications (food, paint, construction products, etc.), and its characterization becomes primordial.
Thus, this work proposes a methodology to automate the size characterization of titanium dioxide particles imaged by scanning electron microscopy (SEM). Today, SEM imaging is widely used in laboratories and manufacturing industries and is considered in metrology as a reference technique capable of reliably determining the size, size distribution and shape of nanoparticles. However, the study of this type of particles remains challenging because of their non-spherical shape and their ability for agglomeration. The commonly used image processing methods such as watershed or active contour lack of generalizability. Indeed, the adjustment of the parameters of such algorithms is almost systematically required and slows down the automation of the processing chain. Moreover, these traditional methods are not efficient when performing segmentation over non smooth convex objects that strongly overlap. Due to this complexity, the characterization of this type of content is not automated and is frequently performed manually by experts in nanometrology.

To overcome this problem, we propose a fully automated data-driven deep learning pipeline for estimating the particle size distribution of SEM samples. This pipeline consists of three key stages: individual particle segmentation, particle agglomeration state classification and particle completion when studied particles are classified as partially imaged.
This methodology paves the way to a better understanding of the studied sample composition. Indeed, combining the particle segmentation with an agglomeration state classification allows to estimate the share of each type of particles in the estimated particle size distribution. To evaluate the performance of the proposed method, we use a test set composed of 19 images (for a total of 3741 particles) and calculate the detection score (84%), the mAP value (60.6) and the Sørensen–Dice coefficient (Sorensen, 1948) (0.95). The results confirm that the proposed approach yields to both accurate and robust segmentation of agglomerated titanium dioxide particles. Using the predicted particle segmentations, scanning electron microscopy sample characterization commonly relies on derived quantities such as the projected equivalent diameter. For this measurand, more than 96 % of measurements show an error of less than 5 % and 51 % of measurements show an error of less than 1 % when tested against ground truths segmentation.

*Intervenant

Deep learning for sparse spectral ptychographic x-ray computed tomography (Spect-PXCT) .

Mohamed Redhouane Boudjehem*[1,2], Anico Kulow[1,2], Florent Magaud[1,2], Jean-Louis Hazemann[1,2], Samy Ould-Chikh[3], Javier Perez[4], and Julio Cesar Da Silva[1,2]

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Résumé

X-ray Ptychography (1) (2) is a coherent diffraction imaging technique. In addition to its capacity to provide images with high resolution and thus allow the study of complex materials, X-ray ptychography can be combined with tomography (3) to provide a 3D reconstruction of a specific sample and thus permit the investigation of the microstructure. The acquisition of ptychographic tomogram can take half a day or more, depending on the size of the sample, the number of projections and the exposure time. Reducing the number of projections and/or the exposure time would reduce the acquisition time, but these solutions will directly affect the resolution and the reconstructed tomogram will be noisy.This problem can be overcome with help of deep learning. Recently, a Generative Adversarial Network (GAN) (4) (5) called TomoGAN (6)(7) was proposed to improve the quality of images obtained by high-resolution tomography. In general, GAN combines two neural networks, a generator (G) and a discriminator (D), which compete in a zero-sum game: G generates candidates that D evaluates; those evaluations serve as feedback to G. TomoGAN model can be trained with limited data, performs well with high-resolution datasets, generates greatly improved reconstructions of low-dose and noisy data, and is very resilient to overfitting. Previous works demonstrated that the number of projections required can be reduced by a factor of at least 8 while keeping high-quality of the reconstructed images.
We will show here, how this technique can be applied to the case of spectral tomography, as an example, we will take 2 tomograms of the same sample recorded at two different energies, taking advantage of the similarity of the tomograms.By training the networks on one complete high-resolution tomographic dataset at a given energy, we are capable to retrieve images from tomographic dataset at another energy with much fewer projections than what would be necessary for the retrieved good-quality images using standard algorithms.

References

(1) Pfeiffer, F. X-ray ptychography. Nature Photon 12, 9–17 (2018).

*Intervenant

LaueNN: Neural network based hkl recognition of Laue spots and its application to polycrystalline materials

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Résumé

A feedforward neural network (FFNN) model is introduced for efficient and accurate prediction of Laue spots hkl in single/multi-grain/multiphase Laue images. Laue microdiffraction is an X-ray scattering technique for the determination of local structural parameters (strain, stress and orientation) in materials from microstructure mapping (2D and 3D). The use of a polychromatic beam offers many experimental advantages (no rotation of the sample, many diffraction spots, signal that can be used even in the presence of strong orientation disorder). However, in the case of polycrystalline microstructures, the determination of the structural parameters (lattice parameters) from the fine analysis of the relative position of the spots requires identifying unambiguously all the spots forming the Laue pattern corresponding to an individual crystal among all other spots. The indexation step of the data analysis must be reliable to input unambiguous experimental dataset to the structural model refinement (final step in analysis) and rapid; since production rate of data on the synchrotron line can amount to several 10000s diffraction images per hour, each Laue image being able to contain contribution from multi-grain/ multi-phase present in the probed volume of the material.

Several approaches have been carried out by different groups allowing to index single crystals (1-2) and polycrystals (for example: XMAS, LaueTools (3-5)). In the latter case, the most time consuming, in the whole data analysis workflow, is the indexation step i.e., determination of Laue spot *hkl* Miller indices from sets of spots related to the probed crystal. To this effect, we propose (6) employing a FFNN based model to tackle the bottleneck of indexation

*Intervenant

Clustering pour Structure de 4Dstem en utilisant NMF

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Résumé

Se différencier d'une série de ED patterns entre savoir et non-savoir phases de crystalline

*Intervenant

Learning the committor probability using data-driven path collective variables

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Résumé

We have developed a new method aimed at predicting the committor probability for a system of two metastable states, focusing on a data-driven generalization of path collective variables(1). In this approach, we perform kernel regression of the committor within a first projection of the Cartesian coordinates onto a subspace formed by CVs. This subspace can be arbitrarily formed, e.g. by selecting a list of typical scalar CVs, or by using more abstract, high-dimensional CVs. The obtained collective variable is a one-dimensional estimation of the committor, which makes for easy comparison of CV subspaces. We apply this methodology to the well-known problem of ion pairing in water, with a focus on NaCl and LiF, and show that better estimators of the committor can be obtained by taking into account information related to the solvent compared to the only interionic distance. (1) 10.1063/1.2432340

*Intervenant

Towards Artificial Neural Networks Exchange and Correlations functionals in Density Functional Theory for Transition Metal Complexes

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Résumé

Recent studies have shown that by training Machine Learning (ML) models with highly accurate ab initio wavefunction data, one can construct exchange and correlation functionals in DFT that improve upon standard approximations. As such, Nagai et al. (2022) demonstrated that Artificial Neural Network (ANN) functionals can yield very accurate values of atomization energy and ionization potential of small molecules consisting of light atoms. Yet, this is an emerging approach in the field of electronic structure calculations and many questions stay open on how to adapt the ML framework to particularly challenging materials or proprieties, such as, for example, transition metal complexes and adiabatic energy differences.

In our work, we propose a combination of ANN and non-gradient bio-inspired training methods adapted from Particle Swarm Algorithm (PSO). By using small trial molecules (H2O and FeO) we find that the method of training is robust and outperforms other non-gradient based trainings reported in the literature. In some cases, the proposed approach of learning energy differences and electronic densities simultaneously does not work locally and the optimization can yield an improved energy at the detriment of the density. This highlights the challenge in defining pertinent loss functions that better fit the desired physico-chemical properties.

*Intervenant

Gold standard finite temperature simulations of materials via machine learning

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Résumé

Density functional theory is the workhorse of materials simulations. Unfortunately, results often fluctuate depending on the specific choice of the exchange-correlation functional and this significantly limits the predictive power of this approach. Coupled-cluster theory, including single, doubles and perturbative triples, is widely considered as the "gold standard" of quantum chemistry as it can achieve chemical accuracy, 1 kcal/mol, for non-strongly correlated applications. Because of the high computational cost, the application of coupled-cluster theory in materials simulations is rare, and this is particularly true if finite-temperature properties are of interest and molecular dynamics simulations have to be performed. By combining recent progress in machine learning models for energy surfaces with low data requirements and in the implementation of coupled-cluster theory for periodic materials, we show that chemically accurate simulations of materials are practical and could become soon significantly widespread. As an example of this numerical approach, we consider the calculation of the enthalpy of adsorption of CO2 in a porous material.

*Intervenant

Prediction of quantum paraelectricity and quantum phase transitions using ab initio self-consistent lattice dynamics

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Résumé

Quantum paraelectric materials are incipient ferroelectrics. They show a strong softening of an optical phonon branch with decreasing temperature, leading to non-linear increase in the dielectric constant. This branch, however, is stabilized by the zero-point motion of the atoms, preventing the phase transition to a ferroelectric phase even at 0 Kelvin. Here, we present a theoretical study of the quantum paraelectric state in KTaO3 and using ab initio quantum self-consistent lattice dynamics. We use a combined density functional theory and machine learning methodology to obtain the temperature dependence of the interatomic force constants.
This allows us to calculate temperature dependent phonon spectra and the softening of the relevant optical branch, which we show to remain stable down to 0 Kelvin. From the phonon spectra we extract the static dielectric constant as a function of temperature, which accurately reproduces experimental values. Additionally, we study the softening and splitting of the phonon modes due to external stimuli like pressure and strain, which in turn allows us to determine the quantum critical points using the stability range of the ferroelectric soft mode. Lastly, we show how to calculate the electrostrictive tensor at finite temperature.

*Intervenant

Latent Langevin models of atomistic dislocation dynamics

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Résumé

Crystal plasticity is controlled by dislocations, line charges of deformation, which form dense networks under sustained deformation or irradiation. Resolving their complex evolution mechanisms under applied stresses requires atomistic simulations, but computational bounds on accesible time and length scales means simulations can have large uncertainties which complicates analysis. Similar issues arise in molecular simulations, and various forms of generative model have recently been proposed as solutions, drawing samples in the latent space of a suitably designed (and trained) autoencoder to reduce variance through bootstrapping. Howver, due to the amount of training data required, it is not clear if these elegant methods can be applied to the large atomistic systems required for dislocation plasticity. I will present an efficient alternative, demonstrating that atomistic descriptor functions typically used to regress energies and forces form an excellent latent space for the construction of multiobjective, data-driven models. Simulation trajectories in this latent space can be used to learn a high dimensional Langevin model, which is able to generate plausible stochastic trajectories which capture complex dislocation phenomena such as yeilding, for low training cost and negligable resampling cost.

*Intervenant

Machine learning interatomic potentials to improve atomic scale description of nuclear fuel materials.

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Résumé

High-accuracy first-principles methods such as Density Functional Theory (DFT) are the approaches of choice for atomic scale characterization of nuclear fuel materials. However due to the high computational cost of these methods, numerous properties cannot be properly studied. At higher-scales, semi-empirical potentials allow molecular dynamic simulations involving up to billions of atoms but usually poorly compare to first-principles reference calculations for crucial properties such as defects formation and migration energies or phonon density of states (1).
In recent years, numerous studies have shown the relevance of machine learning tools to develop accurate interatomic potentials by fitting the potential energy surface (PES) on a consistent set of electronic structure data (2). So-called machine-learning interatomic potentials (MLIP) maintain the accuracy of DFT through large-scale simulations at a fragment of its computational cost.

We developed high dimensional neural network potentials (HDNNP) (3) and spectral neighbour analysis potentials (SNAP) (4) for the U-O system. In order to improve the PES' sampling, we paired state of the art DFT+U calculations with active learning methods. This enabled the generation of a diverse database, on which the potentials are trained. We confront these new potentials with widely used semi-empirical potentials for actinide compounds (CRG (5), Morelon (6), etc.) to highlight the improvements in terms of atomic description of nuclear fuel materials.
(1) M. Jin, M. Khafizov, C. Jiang, S. Zhou, C.A. Marianetti, M.S. Bryan, M.E. Manley, D.H. Hurley, Assessment of
empirical interatomic potential to predict thermal conductivity in ThO2 and UO2, J. Phys. Condens. Matter. 33 (2021)
275402. https://doi.org/10.1088/1361-648X/abdc8f.
(2) Y. Mishin, Machine-learning interatomic potentials for materials science, Acta Mater. 214 (2021) 116980.
https://doi.org/10.1016/j.actamat.2021.116980.
(3) J. Behler, M. Parrinello, Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces,
Phys. Rev. Lett. 98 (2007) 146401. https://doi.org/10.1103/PhysRevLett.98.146401.

*Intervenant

Towards robust characterization of structural defects at the atomic scale: from high-temperature simulations to Atom Probe Tomography

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Résumé

A perfect crystal is a purely theoretical concept. Real-world crystals contain imperfections at the atomic scale - also called defects - which control their mechanical properties. However, the identification and characterization of these defects at the atomic scale remains challenging when atomic positions are strongly disturbed. In such conditions, the concept of structural defect itself becomes ill-defined. This is typical of datasets that are affected by a large intrinsic uncertainty (e.g. experimental atom probe tomography (APT) data), or stochastic variations (e.g. atomistic simulations of high-temperature and/or large strain conditions).
A recently-introduced method enables to generalize the concept of defect by assigning a distorsion score to each atom, based on machine-learning outlier detection (1). The distortion score describes a statistical distance of an atomic environment compared to a distribution of reference structures in the space of atomic descriptors (2). Reference structures can be sampled as defect-free crystals with a certain level of noise, i.e. similar to that in APT reconstructions, or by conducting MD simulations at finite temperature. Based on the distortion scores, we identify structural defects as atoms-outliers deviating from the reference structure.

This work presents the applicability of distortion scores in conjunction with machine-learning methods of structural classification for advanced analysis of defects in metallic systems with elevated levels of noise where conventional geometry-based methods of structural analysis commonly fail, including the structures from finite-temperature and radiation damage simulations and data from APT experiments.

(1) A.M. Goryaeva et al. Nature Comm. 11, 4691 (2020)
(2) F. Musil, et al. Chem. Rev. 121, 9759 (2021).

*Intervenant

Apports de l'IA aux caractérisations des matériaux par spectroscopies de faisceaux d'ions

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Résumé

Les spectroscopies par faisceaux d'ions énergétiques (IBA : Ion Beam Analysis) constituent un ensemble de techniques spectroscopiques qui permet de déterminer la composition chimique en éléments majeurs et traces, légers et lourds, de composés solides. L'IBA est principalement employé en Sciences des Matériaux et en Sciences de la Terre.
Ces spectroscopies sont quantitatives et reposent sur la simulation des spectres issus des rayonnements produits par les interactions entre les projectiles et les atomes du composé. Les rayonnements simultanément collectés sont de différentes natures : particules rétrodiffusées, particules issues de réactions nucléaires, photons X produits par ionisation. Le traitement des données reste fastidieux, d'une part du fait que de nombreux processus physiques doivent être pris en compte dans les simulations, et que d'autre part une cohérence globale entre les spectres issus des différentes voies de réaction est requise.
A partir de bases de données produites par des outils de simulation adaptés, nous avons étudié l'apport de l'apprentissage supervisé auquel nous avons associé l'augmentation artificielle de données pour traiter rapidement et massivement des spectres expérimentaux. Nous avons pu démontrer la faisabilité de la méthode, et nous explorons actuellement la possibilité de chaîner 2 réseaux de neurones : le premier est dédié au classement, afin de déterminer les éléments effectivement présents dans l'échantillon, le second étant destiné à la régression pour reproduire les spectres expérimentaux et accéder ainsi à la quantification de la composition.

*Intervenant

The recourse to artificial intelligence to design Co-free wear-resistant alloys

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Résumé

In order to prevent the activation of 60Co cobalt particles in the primary circuit of nuclear reactors, it is necessary to replace Stellite alloys (CoCrC) used as wear-resistant coatings, with cobalt-free alloys. Different materials have been developed (eg. NOREM or Nitromax alloys) in past decades, but none of them offers a satisfactory set of properties. This project is dedicated to computational design of new Co-free wear-resistant alloys. Both machine learning and physical (thermodynamic) models have been developed and used. These models were integrated in a multi-objective genetic algorithm to optimize chemical compositions, with different sets of objectives and constraints.

A hardness model could be established, using Gaussian process regression, to correlate this property to composition, based on numerous reported experimental data. On the contrary, for the wear resistance model, only a small number of experimental data coming from various sets of conditions of wear measurements, is available. Classical data mining regression tools have failed in this situation of "small and often incomparable data", and a solution was found by using a pair-wise comparison algorithm (SpringRank). First, alloys have been ranked by the pair-wise comparison algorithm; then, their rank has been correlated to alloy composition using Gaussian process regression. Finally, thermodynamic calculation (CALPHAD, Calculation of Phase Diagrams method) was used to predict alloy's structure and phase stability.

The proposed design approach has been experimentally evaluated. Several original alloys have been elaborated and tested (microstructure, hardness, wear and mechanical properties). Their properties globally fulfil the criteria of modelling.

*Intervenant

Rational Composition Optimization: Coupling Mixture Designs, Combinatorial Methods and Machine Learning

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Résumé

Multinary optimization has been at the heart of recent developments, either for High Entropy Alloy or for metallic glasses, amongst others. It represents a challenge that requires overcoming the usual method of "one sample at a time". Combinatorial approaches have been applied many times to N-element systems, and this study proposes to couple it to mixture design, in order to guarantee a uniform and systematic screening of the composition space, by elaborating and characterizing magnetron sputtered films with controlled gradients of composition.
This method was applied to the refractory high entropy alloy system Nb-Ti-Zr-Cr-Mo, on as-grown and annealed samples, as well as on a nitride pseudo-ternary, Ti-Al-Nb-N. The mechanical properties were measured by nanoindentation for both, while crystallinity was assessed using XRD - and EBSD in the case of the HEA. Conductivity measurements were performed on the nitride system. This high-throughput screening resulted in an experimental database covering the properties of 460 HEA compositions and 140 nitride compositions that was used to train Machine Learning models linking compositions, structures and properties.

In order to explore the possibilities offered by Machine Learning, several databases and different models were used. Raw experimental data and statistically processed database allowed delineating the performances of Machine Learning. Models with increasing complexity were tested: multilinear regression with interactions, Support Vector Machine, Random Forest and Neural Network, with previously adjust hyper-parameters. Random Forest and Neural Network show a very good accuracy, either on regression or on classification, for property

*Intervenant

Intelligence artificielle symbolique pour le design de nouveaux matériaux.

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Résumé

La science des matériaux suscite un intérêt grandissant et l'intelligence artificielle (IA) a un rôle à jouer dans l'évolution de ce domaine. L'IA est principalement utilisée pour simuler des phénomènes physico-chimiques ou pour traiter des données expérimentales ou elles-mêmes simulées.
Dans nos travaux, nous nous intéressons à l'application de l'IA symbolique pour l'exploitation des données expérimentales. Par nature, compte tenu de leur coût (humain et financier), la quantité de données est rarement pléthorique. Cela exclut bien souvent les modèles classiques d'IA qui nécessitent un grand nombre de données et qui sont souvent obscurs (on parle de " boites noires "). Cela motive notre utilisation de modèles à base de règles qui sont interprétables par nature.

L'IA symbolique permet d'aborder différentes problématiques offertes par la science des matériaux : la prédiction de propriétés à partir des paramètres du procédé ou à partir des poudres qui sont utilisées, ou encore l'élaboration d'un plan expérimental. Nous nous intéressons dans cette présentation à la prédiction de propriétés à partir des paramètres de fabrication. Nos approches proposent à partir de quelques données expérimentales d'extraire des connaissances qui sont à la fois utiles au chercheur et à la machine pour faire ses prédictions.

Pour cela, nous nous proposons dans un premier temps d'extraire la causalité entre ces paramètres et une propriété. Cela permet non seulement de réduire le nombre de variables, mais également de fournir une indication majeure qu'est un lien causal, sans pour autant faire d'hypothèse sur sa nature (e.g., linéaire).

Ensuite, nous étudions la nature de ce lien causal. Par exemple, entre autres, nous pouvons détecter un lien graduel et donc fournir une règle graduelle de la forme PLUS ... PLUS ... (ou autres variations). Les règles graduelles que nous extrayons ont été évaluées et comparées à d'autres modèles et montrent de meilleures performances que les autres modèles tout en offrant une interprétabilité sans concurrence.
Nous présenterons nos premiers dans ce domaine et quelques résultats afin de montrer que l'IA symbolique a également sa place dans la science des matériaux.

*Intervenant

Modelling NMR Spectroscopy of Oxide Glasses with Machine Learning

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Résumé

Solid-State NMR has now become a key spectroscopy in numerous fields of material sciences. The local environment of each atom is characterized by a NMR fingerprint that can be acquired independently of the crystalline, disordered or vitreous form of the studied material. With recent advances in DFT computations, NMR can now be combined with Molecular Dynamics (MD) simulations to help the interpretation of experimental data. However, such calculations are severely limited in system size by the high-computational cost of DFT computations.
In the last years, machine learning (ML) approaches have emerged as powerful mehods for accelerating MD and computing materials properties with an accuracy and an efficiency that are close to that of DFT methods and classical MD, respectively. In the specific field of solid state NMR, few approaches have been recently proposed that can be applied to oxide glasses which are complex materials which structural features that are still debated. We describe here an approach based on the concept of atomic-centered descriptors (such as SOAP) combined with Kernel Ridge Regression (KRR) or Artificial Neural Network (ANN) techniques. This enables the prediction of NMR properties for structural models of thousands of atoms. An optimal scheme based on the Least-Square Support Vector Regression algorithm will be presented with applications to simple borate and silicate glasses.

*Intervenant

Prediction of disorder potential inside heterostructures using machine learning

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Résumé

We present a machine learning approach that allows to characterize the disorder potential of a two-dimensional electronic system from the electronic transport properties (ETP). We first chose an ETP that is fast to compute but not experimentally observable. However, it allowed us to train a neural network with a large set of disorder configurations and corresponding simulated ETP. We show that the trained network is able to recognize characteristics of the disorder potential of an unknown sample from the ETP, and that the machine-learning approach even allows to reconstruct the complete potential landscape seen by the electrons (1).
In order to determine the disorder potential of a real sample from experimental transport measurements, we are currently working on the recognition of the potential from measured ETP which is the scanning gate spectroscopy. This objective is more challenging due an increased amount of numerical resources needed to create the training data. We propose improvements in the approach to obtain reliable results in spite of a small amount of data used to train the neural network.

(1) : G. J. Percebois and D. Weinmann Phys. Rev. B 104, 075422 (2021)

*Intervenant

Finding and engineering high-conductivity 2D semiconductors from first principles

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Résumé

Thousands of novel 2D materials have been predicted from first-principles, offering exciting perspectives for the design of high-performance electronic devices. We focus here on intrinsic, phonon-limited transport in semiconductors and start from the Materials Cloud's database of 256 exfoliable materials with less than 6 atoms per unit cell.
The most conductive layers are identified by establishing desirable band features based on 2 well-known high-conductivity semiconductors (Phosphorene and InSe). The best candidates are selected, and their conductivity is computed using density-functional perturbation theory and the Boltzmann transport equation. Calculations are done in highly-doped systems, with carrier densities of 10ˆ13 cm-2 induced by field effect. The selected materials' outstanding transport properties are explained via a thorough analysis of electron-phonon scattering (1).

Building on the insights gained in the process, we then discuss pathways to engineer high conductivity in 2D layers with otherwise limited performances. Supported by first-principle calculations, electron-phonon scattering is shown to be suppressed via two mechanisms. Valley-engineering consists in eliminating intervalley scattering by shifting the valleys in energy, using strain or other symmetry-breaking perturbations in selected materials (2). Remote screening designates the screening of electron-phonon interactions in the semiconductor from a neighboring metallic layer within a van der Waals heterostructure, and it is particularly efficient in materials where the Fröhlich interaction dominates (3).

(1) T. Sohier, M. Gibertini and N. Marzari, "Profiling novel high-conductivity 2D semiconductors", 2D Materials 8, 015025 (2020)

(2) T. Sohier, M. Gibertini, D. Campi, G. Pizzi, N. Marzari, "Valley-engineering mobilities in two-dimensional materials", Nano Letters 19, 3723-3729 (2019)
(3) T. Sohier, M. Gibertini, and M. J. Verstraete, "Remote free-carrier screening to boost the mobility of Fröhlich-limited two-dimensional semiconductors", Physical Review Materials 5, 024004 (2021)

*Intervenant

Graph Theory for Molecular Dynamics simulations

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Résumé

Our recent developments in graph theory algorithms applied to molecular dynamics trajectories (DFT-based and classical MD) will be presented.
1 – Graph theory for the automatic recognition of 3D conformers along MD trajectories, at the atomistic granularity level, isomorphism being a key component together with keeping the atoms chemical nature. Isomorphism allows recognize conformations and provides graphs of transitions, the reduction in the isomorphism complexity has been achieved by the introduction of "orbits" and "reference snapshots." The method provides the changes in conformations over time based on hydrogen bond(s), proton transfer(s), coordination number(s), covalent bond(s), fragmentation(s). We will show applications to gas phase molecules and clusters as well as direct transferability to condensed matter.

2 – Graph theory and deep learning for going from the graphs to 3D molecular structures, showing applications to peptides of increasing complexity.

3 – Graph theory for the assignment of anharmonic vibrational modes from MD simulations, building one graph/vibrational mode, without harmonic approximations. Graph vertices are made of the internal coordinates self-contributions to the mode while the graph edges contain the correlations between the internal coordinates. All coupling motions are therefore naturally included in the graph modes. The ultimate advantage of graphs is the capability for comparing graphs and extracting similarities, exactly what is needed for comparing vibrational modes between molecular systems, and this will be illustrated for peptides and their dimers.

4 – Gas phase polymers are highly flexible hence displaying complex dynamics, which analysis in terms of time-evolution of the 3D structures is rather complicated. We have developed graphs algorithms to analyze such trajectories directly in terms of the polymorphism of the H-Bonded rings over time. Illustrations will be given on Z-Ala6 and Gramicidin peptides, to emphasize that this graph level granularity is the only one giving rise to a comprehensive view of the 3D structures time-evolution.

Works done in collaboration with Prof D. Barth, Dr S. Bougueroua, Dr D. Galimberti, Dr M. Bricage, Y. Aboulfath (PhD), V. Chantitch (PhD)

Our publications on these topics:

(1) S. Bougueroua, R. Spezia, S. Pezzotti, S. Vial, F. Quessette, D. Barth, M.-P. Gaigeot,

*Intervenant

Prédiction par une approche de Machine Learning de l'énergie de ségrégation aux joints de grains dans l'aluminium : influence de la symétrie

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Résumé

Cette étude vise à prédire la ségrégation aux joints de grain d'atomes en solution, via le modèle de White et Coghlan (WC). Celui-ci nécessite néanmoins la connaissance précise de l'énergie de ségrégation par site atomique au joint de grain pour chaque joint de grain, et chaque soluté, ce qui s'avère très contraignant à obtenir par les méthodes numériques classiques comme la dynamique moléculaire. Pour pallier cette contrainte, une approche de type Machine Learning a été mise en place, qui permet de prédire l'énergie de ségrégation par site, à partir de la seule structure des joints de grains vierges. La méthode proposée applique une approche de type forêts aléatoires (Extra-Trees) entraînée sur un dataset de 38 joints de grains Σ5 d'aluminium et différents solutés, généré par dynamique moléculaire, moyennant l'introduction d'un nombre limité de descripteurs facilement interprétables, tels les paramètres de Voronoï et de Steinhardt. L'approche ainsi développée fournit des prédictions rapides et précises, en nette amélioration par rapport à une précédente étude (1). De plus, le rôle des descripteurs caractérisant le degrés local de symétrie dans les joints de grain (paramètres de Steinhardt) sur l'amélioration des résultats par rapport à (1) est démontré. Enfin, une caractérisation originale du degrés de symétrie des différents joints de grains est proposée, et mise en relation directe avec la qualité des prédictions de l'approche utilisée dans cette étude. (1) L. Huber & al. (2018), npj Computational Materials, 4(1), 1-8.

*Intervenant

5 Résumé des présentations par posters

An integrated data science approach to ranking the synthesizability of hypothetical zeolites

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Résumé

Zeolites are nanoporous alumino-silicate frameworks widely used as catalysts and adsorbents. Even though millions of siliceous networks can be generated by computer-aided searches, no new hypothetical framework has yet been synthesized. The needle-in-a-haystack problem of finding promising candidates among large databases of predicted structures has intrigued materials scientists for decades; yet, most work to date on the zeolite problem has been limited to intuitive structural descriptors such as distances, angles and ring sizes. In this work, we first analyze the structural motifs in the Deem database of hypothetical zeolites to investigate whether the structural diversity found in this database can be well-represented by these descriptors or whether a more general representation of atomic structure, furnished by the smooth overlap of atomic positions (SOAP) method, is required to capture accurately structure/property relations. We found that SOAP with a cutoff length of 6 Å outperforms the intuitive descriptors in machine-learning the molar energy and volume of the hypothetical framework in the dataset. The first three kernel principal components of the SOAP vectors capture the main variability in the data set, allowing a 3D point cloud visualization of local environments in the Deem database that shows good correlations with the contribution of a given motif to the density and stability of its parent framework. As a second further step, we have developed a rigorous data science scheme, termed the "Zeolite Sorting Hat" that exploits interatomic correlations via the SOAP descriptor to discriminate between real and hypothetical zeolites. This approach also allows to classify zeolites in different compositional classes, thus offering guidance on possible synthetic strategies for a given hypothetical framework. We find that, regardless of the structural descriptor used by the zeolite sorting hat, there remain hypothetical frameworks that are incorrectly classified as real ones, suggesting that they might be good candidates for synthesis. The structural features that distinguish real and hypothetical frameworks emerges as an output of the zeolite sorting hat. Further ranking of the candidates can be achieved based on thermodynamic stability and/or their suitability for the desired applications. Based on thisworkflow, we propose three hypothetical frameworks differing in their molar volume range as the top targets for synthesis, each with a composition suggested by the zeolite sorting hat.

*Intervenant

Application de l'apprentissage automatique pour le développement de nouveaux Matériaux Cimentaires Bas Carbone : une revue bibliographique

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Résumé

L'utilisation de ciments, en tant que matériaux de construction, augmente de façon continue dans toutes les régions du monde. Cependant, la fabrication de clinker, en vue de produire du ciment, est un procédé à forte intensité énergétique et émetteur de CO2. Des ciments de nouvelle génération, dits bas carbone peuvent potentiellement diminuer l'empreinte carbone. Au cours des dernières décennies, l'apprentissage automatique est apparu comme une approche holistique et prometteuse pour prédire les propriétés des matériaux, même sans une compréhension globale des corrélations sous-jacentes entre la composition et les propriétés des matériaux. La présente démarche scientifique consiste à alimenter des algorithmes d'apprentissage automatique par des données d'entrée pour conduire des tâches permettant l'optimisation des propriétés déterminées des matériaux cimentaires consolidés. Dans ce poster, nous présentons des éléments sur l'état de l'art concernant l'application des modèles d'apprentissage automatique dans l'étude des performances des matériaux cimentaires bas carbone.

*Intervenant

Calculation of uncertainties in deep neural networks

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Résumé

In recent years deep learning methods have impacted many scientific disciplines, since they become more and more efficient, and huge amount of data are becoming available to train deep neural networks. In fields as diverse as astrophysics, particle physics, or materials science, data can be provided by physical models or by experiments; both data sources are typically subject to uncertainties, because of the nature of physical phenomena or because of the experimental uncertainty on measures.
Standard deep learning approaches are today hardly capable of considering uncertainties during the network training phase or even to determine the uncertainties on the network predictions. In this poster we will discuss uncertainties of the input data, and envisage possible ways to improve the training phase of neural networks by taking those uncertainties into account. We conclude with an outlook on possible uses of this approach to account for uncertainties, and exploit them, to treat probability density functions with deep learning approaches in experimental and computational materials science.

*Intervenant

Criblage de nouveaux matériaux fonctionnels ESOs

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Résumé

Les oxydes stabilisés par entropie (ESO) sont des oxydes avec un mélange d'éléments métalliques M sur un site cationique d'un oxyde simple. A haute température, ces matériaux sont stabilisés grâce à l'entropie configurationnelle résultante de ce mélange. Les ESO peuvent avoir des propriétés particulières comme une constante diélectrique très élevée. Ils peuvent être utilisés comme catalyseur, supraconducteur et électrolyte dans les batteries au lithium. En considérant un ESO avec un mélange de 5 éléments sur le site M parmi une liste de 16 éléments et en faisant varier leur composition par pas de 1%, on trouve plus de 16 milliards de composés possible pour une structure donnée. Cependant parmi toutes ces possibilités beaucoup ne sont pas stables. Notre travail de recherche consiste ainsi à prédire par calcul et Machine Learning (ML) les combinaisons qui seraient potentiellement stables ou plutôt " stabilisables " par entropie. En collaboration avec un laboratoire qui réalisera la partie expérimentale, notre démarche s'inscrit dans le cadre du projet ANR DETOX qui vise à découvrir de nouveaux ESO. La méthodologie appliquée s'appuie sur plusieurs approches couplées : SQS et DFT pour construire une base d'apprentissage et apprentissage supervisé pour la prédiction. En guise d'illustration, nous réaliserons ces calculs sur des mélanges pseudo-binaires, ternaires, quaternaires et quinaires sur la structure NaCl. Cela permettra de valider la méthode développée. Nous pourrons vérifier si nous arrivons à prédire la métastabilité des ESO qui ont déjà été observés expérimentalement comme le composé (Mg,Co,Ni,Cu,Zn)O, et comparer les valeurs d'enthalpie de mélange des mélanges binaires à quinaires à des données thermodynamiques de la littérature.

*Intervenant

Data-driven Langevin equations from molecular dynamics trajectories

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Résumé

The long time scales associated with rare events, in contrast to the short time scale that is accessible by molecular dynamics (MD) make the precise characterization of transition mechanisms, free energy landscapes, and kinetic rates one of the main challenges of computer simulation. We use short molecular dynamics trajectories to extract accurate thermodynamic and kinetic information. To this end, we train data-driven Langevin models of the dynamics of a system projected on a collective variable. This Langevin model is obtained through the optimization of the parameters of an overdamped Langevin equation using the model likelihood until reproducing in a faithful way a set of MD trajectories. We show that the new approach yields accurate thermodynamic and kinetic information starting from a limited amount of MD data. The new approach is conceptually simple, computationally efficient, and could be applied to diverse problems such as phase transitions, physico-chemical processes in solution, protein-protein interaction, and materials characterization.

*Intervenant

Détection d'objets en microscopie électronique en transmission par modèles d'apprentissage profond

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Résumé

La caractérisation d'objets de taille nanométrique par microscopie électronique à transmission (MET) est essentielle pour prédire et évaluer l'évolution des matériaux. Ces objets, visibles par contraste de phase (nanobulles) ou contraste de diffraction (boucles de dislocation ou précipités cohérents), sont des candidats de choix à l'automatisation. L'analyse manuelle de ces micrographies est souvent fastidieuse, chronophage et non reproductible. Dans ce projet, l'objectif est d'utiliser des outils basés sur les techniques d'apprentissage automatique grâce à des architectures de réseaux de neurones de type Faster R-CNN ou Mask R-CNN. Pour se faire, une première étape de débruitage et de suppression du fond dans les images de microscopie électronique en transmission a été effectué grâce à la technique d'algèbre linéaire appelée décomposition en valeurs singulières. Par ailleurs, l'utilisation de réseaux de neurones pour la détection et la classification d'objets permet d'envisager un comptage plus rapide sans faire de concession sur la précision de celui-ci. Le modèle Mask R-CNN appliqué à des images de microscopie électronique en transmission obtenues sur un alliage à haute entropie apporte par exemple des taux de faux positif et négatif de respectivement 3,2 % et 1,5 % et une précision de 98,12 % par rapport aux annotations apportées à la main pour l'apprentissage. La détection de contours ouvre par ailleurs l'horizon des possibles à l'obtention rapide de paramètres intéressants comme la surface projetée de l'objet, son périmètre, une corrélation spatiale, l'anisotropie élastique du milieu et cetera. Ces quantités physiques peuvent être valorisées dans une optique de caractérisation de matériaux. Le processus sera ultérieurement notamment appliqué à des alliages HEA exposés à différentes conditions d'irradiation pour quantifier l'impact de celles-ci sur la formation du dommage d'irradiation. Dans un second temps, il sera appliqué à des bulles dans UO2 et à des précipités cohérents de chrome dans une matrice de cuivre, pour des applications dans le domaine des nanotechnologies.

*Intervenant

DFT investigation of the very first stages of silicide interface formation during Sputter Growth; low (W/MO) VS High (Ag/Cu) adatom mobylity

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Résumé

Over the years, numerous studies have demonstrated a complex dependence of the film microstructure and the resulting properties on the deposition conditions (i.e. the kinetic energy of the deposited particles, the nature and temperature of the substrate) and the characteristics of the deposited species (surface mobility, chemical reactivity). In this respect, the nature of the interfaces (chemistry, structure, spatial extent and roughness) is anticipated to strongly affect the subsequent film growth.
Understanding the initial growth stages and their influence on the evolution of metallic thin film microstructure (grain size and texture) and properties (stress state, defect density, mechanical properties) is the main objective of the INTEGRAL project funded by the ANR. The central part of this project concerns the implementation of a robust and reliable multi-scale computer modeling of the growth of polycrystalline metallic thin films onto chemical reactive substrate on realistic time scales based on a Monte Carlo Algorithm.

The present contribution is focused on the first step of this multi-scale strategy. i.e. give a comprehensive ab initio study of the elementary mechanisms which occur during the first stages of the growth. We will first characterize silicon (100) substrate the surface reactivity studying the energetic adsorption landscape on for the deposition of tungsten (W) and molybdenum (Mo), as archetype low mobility metal, and silver (Ag) and copper (Cu)) as archetype for high mobility. The most reactive surface sites will then be found will be discussed as well as the possible surface diffusion pathway, and their barrier.
We will also consider the formation of **interfacial silicides layer** that occurs during the early stages of metal growth under energetic conditions. For instance, we will show in the case of Mo the that the incorporation into the Si sublayer is thermodynamically favourable. The role of the concentration of the species introduced in the sub-layer on the stability of the silicide interface will be explored first. Then, the possible formation of an interfacial alloy or phase transition by diffusion of species in the bulk will also be studied. We will conclude with some preliminary KMC results.

[*]Intervenant

Exploring machine learned reaction coordinates in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions

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Résumé

An elementary step of a chemical reaction links two metastable states. The transition mechanism and the time to perform the transition for each of these elementary chemical step is required to better understand the catalytic processes. Direct numerical simulations (DNS) are generally out of reach when using ab initio molecular dynamics (AIMD) because of their computational cost. Dedicated rare event simulation methods have therefore been devised to overcome this limitation. In this work, one of these methods called Adaptive Multilevel Splitting (AMS)1,2 is studied, combined with ab initio molecular dynamics (periodic plane-wave DFT). As many other rare event methods, it requires some information on the progress of the transition, quantified here using a one-dimensional Reaction Coordinate (RC). Determining such a RC challenges chemical intuition for complex systems, which is why we turn instead to machine learning approaches.

*Intervenant

Generating new crystal structures with statistical methods

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Résumé

Our goal is to find a method that would propose candidates for new stable materials. The usual approach to achieve this boils down to performing DFT calculations directly on candidate crystal structures that were obtained by substituting the atoms of one element by others. We are going to employ machine learning methods that rely solely on descriptions of the existing crystal structures to attempt to find new ones. In theory, this might lead to the discovery of new materials of unique topology. The approach will rely heavily on Langevin dynamics, a statistical model for simulating molecular systems. The main difficulty to overcome is tied to the periodicity of the structures. The evaluation for this kind of task is troublesome and is usually made by comparing some metrics of the generated structures with the metrics of the existing structures. These metrics might be some functions of the distributions of inter-atomic distances.

*Intervenant

Graph theory as a powerful tool for the MD trajectories post-processing

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Résumé

In this work, we present two different applications of graph theory. Graph theory from theoretical informatics is widely used to recognize, follow in time, statistically analyze conformations, and characterize the 3D structures in Molecular Dynamics (MD) trajectories. (1) The first application concerns the conformer's exploration. A molecular system is defined as a graph such that vertices represent atoms of the molecular system and edges represent the bonds formed between these atoms (covalent bonds, hydrogen bonds, intermolecular interactions, organometallic interactions etc., depending on the system). The exploration of different conformations can be seen as an exploration of different graph topologies. Hence, two conformations are identical if and only if their corresponding graphs are isomorphic, i.e., the two graphs have the same set of bonds (edges) connected to the same set of atoms type (vertices with the same colour). The use of graph theory methods does not only provide a direct and fast methodology to identify conformers but also allows provide all transitions (interconversion reactions) that have been observed between the different conformers. The developed algorithm has been tested on several molecular systems, from small peptides in the gas phase to complex aqueous interfaces in the condensed phase, passing by clusters in catalysis.
The second application is destinated for vibrational mode assignment. In the context of recognizing, characterizing, and comparing vibrational modes. A proof of principles has been presented in ref. (1) for the IR spectroscopy of gas-phase molecules. The idea is to transform the spectral data into coloured indirect weighted graphs where the vertices are the internal coordinates (IC) that participate in the modes (self-terms), and the edges are the internal coordinates cross-terms in the spectrum reconstruction. One graph is hence obtained per mode/per active IR band. Coloured graphs are used to distinguish the possible IC components participating in the vibrational modes (stretching motions, bending motions, torsional motions, etc.). The weights on the vertices and edges of the graphs respectively provide the percentages of contributions of individual ICs and the pairs of correlated ICs within the vibrational motion. The graphs directly show the number of motions that are participating in each given vibrational mode, whether a vibrational mode is made of coupled or uncoupled internal motions (made of connected elements and disconnected ones), whether a mode is made of localized or (highly) delocalized/collective motions (simply by counting the number of connected components in the graph). The algorithm has been tested on different peptides, such as the model peptide dimer (Ac-Phe-OMe)2.

*Intervenant

High Throughput Experimental Studies of Hard Magnetic Films

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Résumé

Combinatorial studies based on the preparation and characterisation of compositionally graded thin films are being used for the screening and optimization of a range of functional materials, including hard magnetic materials. We recently reported on the use of a set of high throughput scanning characterization techniques (EDX for composition, high field Magneto-Optic-Kerr-Effect (MOKE) for magnetic properties, and XRD for crystal structure) to study sets of compositionally graded Fe-Pt films treated to different post-deposition annealing conditions (1). This high-throughput experimental approach is now being used to study the effect of element substitution in Rare Earth - Transition Metal hard magnetic phases (2-14-1, 1-5, 1-12), to reduce dependence of critical REs and to address the RE-balance problem. Beyond optimising known hard magnetic systems, it holds the potential to discover new hard magnetic phases. A variable temperature high field scanning MOKE system is presently being developed at Institut Néel, which will expand the types of data sets we can produce for hard magnetic films (coercivity vs T, Curie temperature, spin-reorientation temperature), but will also extend its use to the high throughput characterization of other functional magnetic materials (e.g. magnetocaloric materials). AI-approaches are now needed for efficient analysis of the data sets we are creating and for data-driven machine learning design of magnets and magnetocaloric materials.
(1) Yuan Hong, Isabelle de Moraes, Gabriel Gomez Eslava, Stéphane Greniea, Edith Bellet-Amalric, Andre Dias, Marlio Bonfim, Laurent Ranno, Thibaut Devillers and Nora M.Dempsey, A high throughput study of both compositionally graded and homogeneous Fe–Pt thin films, Journal of Materials Research and Technology 18 (2022) 1245

*Intervenant

Hybrid ab initio-machine learning simulation of dislocation-defect interactions in tungsten

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Résumé

Calculations of dislocation-defect interactions are essential to model metallic strength, but the required system sizes are at or beyond *ab initio* limits. Current estimates thus have extrapolation or finite size errors that are very challenging to quantify. Hybrid methods offer a solution, embedding small *ab initio* simulations in an empirical medium. However, current implementations can only match mild elastic deformations at the *ab initio* boundary. We describe a robust method to employ linear-in-descriptor machine learning potentials as a highly flexible embedding medium, precisely matching dislocation migration pathways whilst keeping at least the elastic properties constant. This advanced coupling allows dislocations to cross the *ab initio* boundary in fully three dimensional defect geometries. Investigating helium and vacancy segregation to edge and screw dislocations in tungsten, we find long-range relaxations qualitatively change impurity-induced core reconstructions compared to those in short periodic supercells. Our approach opens a vast range of mechanisms to *ab initio* investigation and provides new reference data to both validate and improve interatomic potentials.

*Intervenant

Identification de lois de plasticité cristalline par jumeau numérique et apprentissage statistique

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Résumé

Les matériaux polycristallins sont sujets à des mécanismes de déformations complexes mettant à défaut les modèles mécaniques macroscopiques couramment employés. L'étude de ces mécanismes est à l'origine du développement de lois de comportement microscopiques, permettant une description physique fine de la déformation à une échelle locale, faisant intervenir de nombreux paramètres. La calibration de ces modèles à partir de simulations numériques et de données expérimentales à l'échelle microscopique, et pas uniquement macroscopique, est une question essentielle.
Les progrès réalisés en imagerie des matériaux par rayonnement synchrotron permettent de suivre, au cours d'un essai mécanique, l'évolution de grandeurs internes telles que l'orientation et les composantes du tenseur de déformation élastique (1), à la fois moyennés par grains (Diffraction Contrast Tomography et 3D X-Ray Diffraction) mais également à des échelles 10 à 100 fois plus résolues (scanning-3DXRD).

Parallèlement, les progrès réalisés en terme de simulation numérique autour des méthodes FFT (2) offrent la possibilité de réaliser des simulations de grande taille jusqu'ici inenvisageables par des codes éléments-finis standards.

Les travaux menés visent à combiner ces deux approches par le biais de méthodes d'apprentissage statistique dans le but d'optimiser l'identification des paramètres sur les mesures expérimentales, à différentes échelles. L'ajustement des paramètres à partir de données expérimentales obtenues à des résolutions de plus en plus fines permet également d'évaluer des incertitudes associées à chacun d'eux. La stratégie déployée consiste à " apprendre " le lien entre les contraintes à différentes échelles, afin d'éviter la réalisation de simulations à haute résolution (0.1 à 0.01 μm). Il s'agit d'une méthode de super-résolution micromécanique par un modèle autoencodeur multimodal (3), visant à prédire un état de contrainte fortement résolu à partir de la morphologie et de l'orientation des grains ainsi que d'un état de contraintes faiblement résolu.

(1) Henry Proudhon, Maxime Pelerin, Andrew King, Wolfgang Ludwig. In situ 4D mechanical testing of structural materials: The data challenge. Current Opinion in Solid State and Materials Science, Volume 24, Issue 4, 2020, 100834, ISSN 1359-0286.

*Intervenant

Learning High-level Features for the classification of Small Angle X-ray Scattering nanoparticles data

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Résumé

Small Angle Scaterring (SAS) methods are widely used for analyzing the shape and size of nanoparticles. Analysing the data obtained by these techniques can be very challenging, owing to the indirect nature of the measurement. A multitude of models describing the SAS intensity resulting from nanoparticle of various shapes have been developed by the scientific community and are available in open source packages. The aim of this presentation is to demonstrate that a machine learning approach based on supervised representation learning is effective at guiding the analyst in his choice of model for SAS data analysis. In this work, a simulated SAXS curves database has been generated to train and test different nanoparticle model selection algorithms. This database is used to compare well-known ML classifiers: k-nearest neighborhood (KNN), random forest (RF) and gradient boosting (XGBoost) classifiers. Several combinations of data pre-processing are proposed to normalize the input values. When the data is represented in (I, q) space, classifier have pain to make difference too similar to models. Different space transformation, from simple integration of the intensity curves to supervised deep learning transformation, are designed to optimize the classification performances and we show that all classifiers perform significantly better on some of the new spaces.

*Intervenant

Machine learning quantum Monte Carlo: application to water clusters

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Résumé

A complete understanding of the hydrogen bond and proton transfer mechanism in water is still lacking, since it requires an accurate potential energy surface (PES) on the top of which exceedingly long quantum mechanical simulations of water clusters dynamics are necessary. Reproducing this high-dimensional surface with current high-level computational chemistry methods such as coupled cluster is infeasible for the largest clusters. We test the gradient-based kernel ridge regression methods to reproduce the PES starting from a dataset of energies and forces of the protonated water hexamer obtained via simulations combining classical molecular dynamics (MD) for the nuclei and quantum Monte Carlo (QMC) for the electrons. The QMC+MD approach yields very accurate results, which are however affected by the intrinsic noise inherent in the stochastic sampling of both nuclear and electronic phase space. Despite the intrinsic noise, QMC energies and forces can be successfully machine learned and the derived force field can be used to run long and reliable molecular dynamics simulations.

*Intervenant

Machine-learning approach to model interatomic interactions and vibrational spectrum of titanium carbide

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Résumé

At the macroscopic scale, titanium carbide is known to be an extremely hard refractory and resistant to corrosion ceramic. As such, this material is employed in cutting tools or mixed with other materials to increase the hardiness (1).
At the nanometric scale, titanium carbide exhibits interesting catalytic properties so that it is considered as a replacement for precious metals in certain applications (2). However, controlling its properties requieres a better understanding of its structure and chemical activity at the atomistic scale. For that purpose, while numerous DFT studies have already been performed (3), it becomes timely to develop a precise interaction potential that should enable for large scale simulations.

In this work, neural network potentials are generated using N2P2 (4) with molecular dynamics data from previous DFT calculations on three different nanoparticles: Ti_14C_13, Ti_18C_14 and Ti_18C_18 (5). After obtaining accurate models for each system, we carefully studied the possibilities and limitations of our models especially in terms of accuracy and transferability. Particular interest was set on vibrational properties of the nanoparticles. Vibrational spectra are calculated through Fourier Transform of Velocity Autocorrelation Function which are extracted from molecular dynamics performed using the obtained Machine Learning Interatomic Potential in good agreement with those obtained using Ab initio methods.

References

(1) S.T. Oyama, (1992) "Preparation and catalytic properties of transition metal carbides and nitrides", Catalysis Today, 15, 2, 179-200

(2) F. Viñes, C. Sousa, P. Liu & J. A. Rodriguez viñes, (2005) "A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides" J. Chem. Phys. 122, 174709

*Intervenant

Machine-Learning Based on Regression for the Prediction of NMR Parameters in Zeolites

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Résumé

Machine Learning (ML) approaches are rapidly developed since few years for their applications in science. In particular, applications of ML models, trained on computed physicochemical or biological properties, attract the researchers interest because of their capability to accelerate the theoretical calculations.
In this presentation we will discuss our recent results on the performance of regression-based ML methods to predict NMR isotropic shielding values in a series of zeolites. To assure a heterogenic set of atomic environments, we built a data set that contains aluminosilicate crystals with various out-of-frame ions. These crystal structures were taken from the International Zeolite database (IZA). In addition, zeolites containing the organic-structure-directing agents were included in the data set. Thus, the zeolite dataset comprises Si, Al, O, H, C, F and Li atomic environments. In this study we apply two ML methods (KRR: Kernel Ridge Regression and GBR:Gradient Boosting Regression) with SOAP descriptors as input. The NMR shielding values were computed with PBE exchange-correlation functional for the optimized zeolite geometries and GIPAW method. The ML models were applied to all atoms in the zeolite data set (14,513 atomic environments) and to the
silicon atoms only (3756 atomic environments).
The distribution of the differences between the DFT computed NMR parameters and the predicted by KRR and GBR models for all atoms (see Fig.) revealed very good performance of both regression models. Similar results were obtained when considering a smaller set containing Si atoms. Only one outlier was established with KRR model for both data sets. The mean and standard deviation errors are $<$ 0.6 ppm, which reveals a very promising performance of both regression methods. The training and prediction are faster with GBR than with KRR ML model. We therefore concluded that GBR ML scales better than KRR one.

*Intervenant

Non-supervised deep learning algorithm to improve quality of X-ray computed tomography images

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Résumé

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X-ray computed tomography is a common method for gaining insights into the structure of a material. In order to have high-quality images, it needs a long exposition time and a large number of projections (around half a day per acquisition). Reducing the number of projection or exposition time results in noisy data and reduce the quality of reconstructed images. Deep learning is becoming a common solution to improve the quality of images. TomoGAN(1) is a GAN (Generative Adversarial Networks) type deep learning model created to improve the quality of computed tomography. It required little data to train, and improve greatly the quality of a low resolution or a noisy image. It consists of 2 different models: a generator and a discriminator. Both models are trained together, the generator creates an image based on a noisy image and the discriminator determines if this image is real or fake. The generator is a variation of U-net and the discriminator is a CNN network. Here, we will present our first successful tests of the application of this model on propagation-based phase-contrast X-ray computed tomography of metal alloys. By training the networks on one complete high-resolution tomographic dataset, we are capable to retrieve high resolution images from tomographic dataset with much fewer projections than what would be necessary for the retrieved good-quality images using standard algorithms.

• Zhengchun Liu, Tekin Bicer, Rajkumar Kettimuthu, and Ian Foster, "Deep Learning Accelerated Light Source Experiments," 2019 IEEE/ACM Third Workshop on Deep Learning on Supercomputers (DLS), Denver, CO, USA, 2019, pp. 20-28, doi: 10.1109/DLS49591.2019.00008.

*Intervenant

On the use of Deep Neural Network Potentials for crystallization in Ag-Au nanoalloys

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Résumé

The unique properties of metallic nanoparticles make their study a topic of choice. In particular, bimetallic Ag-Au nanoalloys are being investigated as electrocatalysts to enhance the production of valuable chemicals. However, the chemical properties of these bimetallic nanoparticles are very dependent on their morphology, size, and atomic composition. Fine control of the nanostructure significantly impacts the nanomaterial catalytic function. For instance, it would be highly insightful to perform crystallization simulations with a large number of atoms over a long period of time, while keeping the accuracy of quantum-based simulations. Until recently, computational physics did not have the tools to meet these specifications without prohibitively high computational costs. In the last few years, we have seen the development of multiple Machine Learning techniques that allow for more efficient and accurate atomistic potentials. Here, we present Deep Neural Network Potentials (DNPs) for Ag-Au systems. We built an extensive DFT database to train these DNPs, consisting of bulk, surface, and amorphous configurations. We validated these DNPs by comparing calculated material properties with DFT results for five unique Ag-Au stoichiometries. Validation tests focused on crystal properties, such as: lattice parameters, bulk and surface energies, and elastic properties. In addition, we also verified the model accuracy in the liquid/amorphous regime. This work will lead to further elucidation of the connection between tailored Ag-Au structures and catalytic activity.

*Intervenant

Path sum: a new way to calculate the ordered exponential of a time dependent matrix

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Résumé

Recently, we have applied for the very first time the concept of Path Sum (Giscard, 2015, J. Math. Phys.) to Nuclear Magnetic Resonance (NMR) (Giscard & Bonhomme, 2020, Phys. Rev. Res.). It allows to explicit the analytical, convergent and non perturbative solution of the Liouville-von Neumann equation encountered in spin dynamics. It is based on graph theory and resummation of walks on graphs on graphs (algebraic combinatorics). The ordered exponential corresponds then to a finite number of operations on a continuous fraction. This approach is highly suitable for analytical results but can also be implemented numerically (with a priori better efficiency that the traditional Zassenhaus approach). Nevetheless, the extraction of simple cycles and walks on a given graph grows exponentially with the the size of the graph (i.e. the size of the associated Hamiltonian). We are curious to discuss with IA/ML experts on that particular topic...

*Intervenant

Physical LassoLars Interaction Potentials

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Résumé

Machine-learning interaction potentials (MLIP) have been recently proposed to bridge the gap between quantum accurate calculations and fast empirical modeling. The main principle consists in using a large set of quantum-accurate calculations to adjust the parameters of a universal mathematical formulation that should represent the interaction potential. Lots of different approaches have been proposed including Artificial Neural Networks, Gaussian approximation potentials, Linearized potentials, Spectral Neighbor Analysis Potential, Symmetric Gradient Domain Machine learning, and Moment Tensor Potentials. The success of those machine-learning interaction potentials (MLIP) is seen through the large variety of materials that were studied including pure metals, organic molecules, water, amorphous materials, and hybrid perovskites. The main issue related to the current MLIP methods that are often designated as "black boxes" is the lack of physical and chemical interpretability of the obtained potential. In this contribution, we will present an alternative machine-learning method that we are currently developing and that is named Physical LassoLars Interaction Potential (PLIP). It combines a physically motivated mathematical formulation for the potential and a constrained linear regression. We will illustrate results on three different materials namely Silica, Gold-iron, and Zinc oxides

*Intervenant

Prédictions de la stabilité et des propriétés électroniques de phases Heusler quaternaires par apprentissage automatique

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Résumé

Les alliages d'Heusler $L2_1$ présentent un intérêt pour divers domaines de recherche comme la thermoélectricité, la spintronique, le photovoltaïque, etc. Généralement étudiés dans des systèmes ternaires, ils peuvent également exister sous équilibre quaternaire pour des applications spécifiques, augmentant l'espace des champs de compositions qui ne peuvent être balayés par des approches de criblages traditionnelles. Il est donc naturel de se tourner vers des méthodes d'apprentissage automatique (*machine learning*) pour accélérer la recherche dans la découverte de nouvelles compositions pertinentes.
De prototype Cu2MnAl, la phase Heusler $X2YZ$ est décrite dans une structure cristallographique du groupe d'espace *Fm-3m*, avec X et Y des métaux de transition et Z un élément du bloc p. Le site $8c$ contenant X peut être séparé en deux sites distincts par un abaissement de symétrie dans le groupe *F-43m*, engendrant quatre positions de Wyckoff, $4a$, $4b$, $4c$ et $4d$, propices à des mélanges quaternaires.

L'objectif de notre étude est de trouver des nouveaux composés Heusler quaternaires qui pourraient exister avec 24 éléments sélectionnés dans le tableau périodique. Pour étudier les propriétés thermodynamiques, électroniques et magnétiques, les calculs premier-principes par DFT sont un allié de choix que nous avons utilisés. En revanche, la combinatoire de notre système engendre 24^4 = 331 776 configurations possibles, soit un nombre trop important de composés pour être étudiée de façon systématique par calculs DFT.

Dans notre travail, une base de données contenant des sous-systèmes de l'ensemble global a été construite, répertoriant notamment des propriétés liées à la structure électronique des composés telles que l'enthalpie de formation et la densité d'état au niveau de Fermi (caractère métallique ou semiconducteur). Nous avons construit un apprentissage supervisé avec le modèle de réseau de neurones afin de prédire les propriétés ciblées des composés quaternaires. Démontrant des performances comparables ou supérieures à celles de la littérature, notre étude permet de faire un criblage sélectif des composés à étudier, et permet de progresser plus rapidement dans la recherche de nouveaux matériaux.

*Intervenant

Sequential Optimization of a Heterogeneous Catalytic Reaction

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Résumé

The development of a novel heterogeneous catalyst that maximizes the yield of a reaction of interest requires optimizing several parameters. These parameters range from the physico-chemical properties of the catalyst itself to the experimental conditions of the reaction in which it is used spanning different time-space scales. In a heterogeneously-catalysed reaction, it is a priori not possible to predict how a change in almost any parameter influences the yield. Therefore, chemists rely heavily on experience and generally on a so-called "trial and error" approach. In this work, we report a sequential bayesian optimization procedure of a yield function that depends on one specific parameter: the residence time of the reactant in the reactor. We apply this approach to the yield function resulting from the simulation of the kinetics of the partial oxidation of isobutene to methacrolein and methacrylic acid. The proposed approach succeeds in finding the optimal isobutene residence time within a reasonable budget limited to a few experiments. Furthermore, we show that the implemented bayesian optimization method behaves properly. Among other parameters the choice of the so-called acquisition function is crucial, e.g. the upper confidence bound, expected improvement, or probability of improvement. It appears that the upper confidence bound and expected improvement needs a cheaper budget, i.e. fewer iterations, than the probability of improvement. Sequential bayesian optimization represents an efficient quantitative approach which is an alternative to a "trial and error" procedure that would be based on the chemist's expertise only.

*Intervenant

Solving inverse problems with deep learning: application to strain profile retrieval in disordered crystals using X-ray diffraction

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Résumé

The determination of crystal-structure information (real space) from X-ray diffraction -XRD- data (reciprocal space) is plagued by the so-called phase problem. Indeed, the absolute atomic coordinates, including deviations from the perfect crystalline structure, affect the complex valued scattered amplitude, whereas the quantity measured in an actual XRD experiment is the intensity, i.e. the square modulus of the amplitude. Hence, whereas the modulus of the amplitude can be straightforwardly determined, the phase is lost in the experiment. Consequently, a direct inversion of the diffracted intensity only provides position-differences, from which there is no direct way to retrieve absolute atomic positions.

For decades, scientists have relied on modeling and fitting algorithms to circumvent this issue: a structural model is used to compute the diffracted intensity and the parameters of the model are refined until a good agreement with experimental data is achieved. Although this method works well for simple problems, it becomes tedious and time consuming for more complex situations.

In this work we focus on ion-irradiated single crystals. These materials are used to model the behavior of materials submitted to harsh radiative environments (spatial or nuclear applications) or materials submitted to ion-implantation (e.g. in the semi-conductor industry). Such crystals exhibit sub-surface lattice strain depth-profiles that determine the macroscopic evolution of the materials, and the accurate determination of these profiles is therefore of critical importance. We here demonstrate that deep convolutional neural networks (CNNs) can be efficiently used to retrieve such strain distributions in crystals: whereas conventional fitting-based methods require a few minutes to several hours to retrieve a strain profile from a single XRD curve, CNNs operate in times ranging from 0.001 to 0.1 sec. Defining the accuracy as the proportion of data exhibiting root-mean-square errors on the strain less than 10%, the best accuracy reaches 71 – 81% depending on the nature of the problem (low strain vs. high strain regimes).

*Intervenant

Adsorption d'atomes d'hydrogène et d'oxygène à la surface de l'intermétallique Al13Co4: apprentissage et transférabilité

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Résumé

Les quasicristaux et les phases approximantes présentent des propriétés de surface originales par rapport aux alliages classiques. Outre la grande dureté, résistance au frottement ou non mouillabilité, la réactivité chimique particulière de ces matériaux offre des perspectives intéressantes (1). La compréhension des interactions de surface avec l'environnement requiert la connaissance des propriétés d'adsorption de ces surfaces, généralement déterminées en utilisant la théorie de la fonctionnelle de la densité (DFT), méthode coûteuse en temps de calcul (2). Dans ce travail, nous avons mis en place un modèle d'apprentissage automatique afin de prédire les énergies d'adsorption de surfaces complexes. Ainsi, le paysage énergétique de l'ensemble de la surface peut être décrit à partir du calcul de l'énergie d'adsorption sur quelques positions, réduisant drastiquement le coût en temps de calcul de ce type d'étude. On applique l'approche décrite ci-dessus successivement aux surfaces (100), (010) et (-201) de l'approximant quasicristallin Al13Co4. On montre que l'on peut réduire d'un facteur 4 le nombre de calculs nécessaires pour décrire de façon correcte les propriétés d'adsorption de ces surfaces (racine carré de l'erreur quadratique moyenne (RMSE) comprise entre 0,1 eV et 0,01 eV selon l'espèce adsorbée). On examine ensuite la possibilité de pouvoir prédire les énergies d'adsorption sur une orientation de surface donnée, à partir des données obtenues sur une autre orientation. Cette approche utilise la notion de transférabilité de l'information disponible dans les différentes bases.

Ce travail ouvre la perspective de réduire considérablement le nombre d'optimisations à réaliser pour déterminer les paysages énergétiques de surfaces de composés complexes.

(1) J.-M. Dubois, Properties and applications of quasicrystals and complex metallic alloys, *Chem. Soc. Rev.*, 2012, 41, 6760-6777
(2) E. Gaudry et al., Catalytic activation of a non-noble intermetallic surface through nanostructuration under hydrogenation conditions revealed by atomistic thermodynamics, *J. Mater. Chem. A*, 2020,8, 7422-7431

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