Journées Plénières IAMAT

2- 5 juin 2026

ENSAM – Aix-en-Provence

Programme

(v1 – 04/05/2026)

Mardi 2 juin 2026 – Après-midi

13h00 – 14h00
Accueil café

14h00 – 14h15
Ouverture des journées

Session 1 : Potentiels Machine Learning – 1

14h15 – 14h50
Timothée Devergne (ORAL INVITÉ)
Slow dynamical modes from static averages

14h50 – 15h10
Didier Bathellier
Les potentiels interatomiques numériques pour l'étude des plasmas

15h10 – 15h30
Luca Brugnoli
Overcoming Sampling Limitations in Water-in-Salt Electrolytes with Fine-Tuned Foundation Machine-Learned Interatomic Potentials

15h30 – 15h50
Evgenii Iablonovskii
Machine-learned potentials for amorphous and crystalline silica/water interfaces

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15h50 – 16h20 : Pause-café

16h20 – 16h40
Magali Benoit
Controlled Diffusion of Ag+ Ions in Silica Matrices: A Machine Learning Approach for Innovative Antimicrobial Coatings

16h40 – 17h00
Stefano Ferrero
Carbon mineralisation at the forsterite–water/CO_2 interface under extreme conditions

17h00 – 17h20
Arnaud Allera
Ab initio accurate entropic and quantum contributions to dislocation glide using machine learning potentials

Mercredi 3 juin 2026 – Matin

Session 2 : IA et Données Expérimentales – 1

09h00 – 09h35
Ewen Bellec (ORAL INVITÉ)
X-ray strain microscopy, Coherent Diffraction Imaging and Machine Learning at the ESRF synchrotron

09h35 – 09h55
Francesco La Porta
Automated Multi-Element composition analysis of X-Ray Fluorescence Spectra via Vision Transformers

09h55 – 10h15
Faycal Adrar
Integrating Machine Learning with X-ray Hyperspectral Imaging for Robust Phase Mapping of Cycled Sodium-Ion Cathodes

10h15 – 10h35
Michel Devel
Physically constrained neural networks for inverse spectroscopy of soot-like carbon nanoparticles from UV–visible spectra

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10h35 – 11h05 : Pause-café

Session 3 : Méta-modèles et Incertitudes

11h05 – 11h40
Amandine Marrel (ORAL INVITÉ)
Uncertainty quantification for numerical simulation : sensitivity analysis, surrogate modeling, and applications in safety assessment

11h40 – 12h00
Marius Duvillard
Apprentissage guidé par la physique pour l'homogénéisation en viscoélasticité : loi effective et champs locaux

12h00 – 12h20
Mattia Ragni
Physics constrained NMR tensor prediction: leveraging differentiation learning in equivariant graph neural networks

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12h20 – 14h15 : Déjeuner

Mercredi 3 juin 2026 – Après-midi

Session 4 : Base de données et Workflow

14h15 – 14h35
Emmanuel Farhi
SHARPES, a data base to hold ARPES dispersions

14h35 – 14h55
Lionel Desgranges
Du spectre Raman à son interprétation par I.A. : le projet Raqoon

14h55 – 15h15
Davide Piccinelli
Multi-Fidelity Gaussian Process Regression for Modeling the Thermal Properties of MOX Nuclear Fuel

15h15 – 16h00
Présentations Flash des posters

16h00 – 16h15 : Pause-café

16h15 – 18h00 : Session Posters

1	**Noémie Djerian**	*Enhancement of nuclear fuel images using artificial intelligence methods*
2	**Faris Flaifil**	*ChatMLIPs MCP: A Model Context Protocol Server for Atomistic Simulation*
3	**Georg Daniel Förster**	*Learning interatomic potentials from finite-temperature properties*
4	**Giorgio Galimberti**	*Atomistic quantification of defect-induced thermal conductivity degradation in UO_2 and implications for fuel performance modelling*
5	**Baptiste Kerleguer**	*Multi-Fidelity Regression for Equation of State Prediction: Bridging Quantum Molecular Dynamics and Semi-Classical Simulations*
6	**Hugo Kuentz**	*High-Throughput Combinatorial Materials Analysis Combining XRD Denoising (U-Net) and Machine Learning: Application to Doped BCTZ*
7	**Marie Landeiro Dos Reis**	*Charged vacancy in Cr_2O_3*
8	**Hoang-Duc Le-Vu**	*Towards Transferable Machine Learning Interatomic Potentials in Hybrid Systems via Component-based Framework for Cross-domain Energy Consistency*
9	**Isabelle Maurin**	*Mutimodal approaches to capture the reaction pathway to the (MgCoNiCuZn)O high-entropy oxide: evidence for spinel intermediates from time-resolved x-ray diffraction and x-ray absorption spectroscopy*
10	**Hayat Ouaissa**	*Bio-inspired optimization and run length encoding for the design of electromagnetic invisibility cloaks*
11	**Zhaxi Pengmao**	*Assessing the capabilities of foundation models to describe interstitial solutes in BCC metals*
12	**Fanny Raison**	*DFT/ML framework for fundamental studies of Laves Phases*
13	**Loan Renaud**	*Dual quantum locking: Dynamic coupling of hydrogen and water sublattices in hydrogen filled ice*
14	**Régis Santet**	*DFT+U computations of strongly correlated systems: the case of PuO_2*
15	**Arthur Souesme**	*Algorithme d'apprentissage profond pour l'analyse haut-débit de données de diffraction des rayons X : Études in situ de la cristallisation à haute température du spinelle $MgAl_2O_4$ dans un système complexe polyphasé d'alumines de transition*
16	**Zhiyi Wang**	*Atomistic Investigation of Martensitic Transformations in Cu-Based Shape Memory Alloys Using Machine-Learned Interatomic Potentials*
17	**Steve Dave Wansi Wendji**	*Machine-Learning Interatomic Potentials for Silver Nanoparticles Embedded in a Silica Matrix*

18h00 – 20h00 : Cocktail

Jeudi 4 juin 2026 – Matin

Session 5 : IA et Données expérimentales – 2

09h00 – 09h35
Zineb Saghi (ORAL INVITÉ)
Application of deep learning in analytical electron tomography

09h35 – 09h55
Pierre Mignon
Simulation of STM Surface Images from Atomic Structures: a Unet-based ML Tool.

09h55 – 10h15
Victor Barrere
Deep learning analysis of HRTEM images for structural characterization of AgCo nanoalloys

10h15 – 10h35
Colin Bousige
Understanding the nucleation and growth of borophene on substrate using Machine Learning tools

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10h35 – 11h05 : Pause-café

Session 6 : Bases de données et Infrastructures Scientifiques

11h05 – 11h40
Thierry Deutsch (ORAL INVITÉ)
Plateforme DIAMOND-DM

11h40 – 12h00
Joao Paulo Almeida De Mendonça
DIAMOND-CW: Container Solutions for Codes and Workflows in Materials Science

12h00 – 12h20
Shoeb Athar
Garbage In, AI Out: High-Fidelity Data Curation for Generalizable Machine Learning in Thermoelectrics

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12h20 – 14h15 : Déjeuner

Jeudi 4 juin 2026 – Après-midi

Session 7 : Potentiels Machine Learning – 2

14h15 – 14h50
Petr Grigorev (ORAL INVITÉ)
Hybrid ab initio-machine learning methods

14h50 – 15h10
Zacharie Waysenson
From MD to Capacitance: Advances in Supercapacitor Modeling with Flexible, Disordered Electrodes

15h10 – 15h30
François Bottin
Ab initio simulations accelerated by Machine Learning

15h30 – 15h50
Georgios Sotiropoulos
Contrastive Regularization of Machine Learning Potentials

15h50 – 16h20 : Pause-café

16h20 – 16h40
Sophie Stibac
Machine Learning Interatomic Potential for the binary W–Cu system in view of modelling a metallic interface

16h40 – 17h00
Edoardo Brando
Machine learning potential of U-Si-Al

17h00 – 17h20
Raynol Dsousa
Towards a multiscale model for simulating materials irradiation using machine learning

Vendredi 5 juin 2026 – Matin

Session 8 : Thermodynamique et Transport

09h00 – 09h35
Guillaume Deffresnes (ORAL INVITÉ)
Data-driven thermodynamics of metallic liquids and alloy design for thermal energy storage

09h35 – 09h55
Baptiste Bernard
The PULSE method to estimate the thermodynamic properties of chemically disordered materials with generative machine learning

09h55 – 10h15
Sonia Salomoni
Pressure–Temperature phase diagram and λ-transition in liquid sulfur

10h15 – 10h35
Shubham Tyagi
Machine-Learning Discovery of Extreme Coherent Thermal Transport Governed by Motif-Level Order in Si/Ge Superlattices

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10h35 – 11h05 : Pause-café

Session 9 : IA et données expérimentales – 3

11h05 – 11h40
Alexandre Boulle (ORAL INVITÉ)
Réseaux de neurones profonds pour l'analyse de données de diffraction des rayons X : principes et applications

11h40 – 12h00
Giovanni Trezza
Full Equivariance in Score-Based Generative Models Towards Molecules and Materials Inverse Design

12h00 – 12h20
Martin Uhrin
Backpropagating through Nature: Building a Differentiable Universe for Materials Discovery

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12h20 – 13h00 : Clôture
