Atelier Méthodes Machine Learning pour la modélisation des matériaux
Toulouse, 22-24 septembre 2021

Programme

SESSION 1 - Mercredi 22 septembre après midi

13h00-13h30	**Introduction**
13h30-14h10	**Oratrice invitée : Clémence CORMINBOEUF** (visio), EPFL, Lausanne Data-driven Approaches to the Discovery and Classification of Homogeneous Catalysts
14h10-14h40	**O1- F.X. COUDERT** (visio), IRCP, Paris Speeding Up the Discovery of Frameworks Materials with Targeted Properties by Machine Learning
14h40-15h10	**O2- N. MINGO**, CEA-LITEN, Grenoble Modeling oxide mixed phases via machine-learning enhanced ab initio calculations
15h10-15h30	*PAUSE café*
15h30-16h00	**O3- B. CASIER**, LPCT, Nancy Hybrid localized graph kernel for machine learning energy-related properties of molecules and solids
16h00-16h30	**O4- G. FRAPPER** (visio), IC2MP, Poitiers Algorithme évolutionnaire auto-apprenant pour la prédiction de nouveaux matériaux : USPEX & ses applications
16h30-17h00	**O5- G.M. DONGHO-NGUIMDO**, IC2MP, Poitiers Prediction of novel Yttrium Nitride phases under pressure

SESSION 2 – Jeudi 23 septembre matin

9h-9h40	**Orateur invité : Frank SMALLENBURG**, LPS, Orsay Linking local structure and dynamics in glassy fluids using machine learning
9h40-10h10	**O6- J. LAM**, CEMES-CNRS, Toulouse Zinc oxide crystallization modeled with machine-learning interatomic potential
10h10–10h40	**O7- R. LOT**, LAAS-CNRS, Toulouse Evaluation of Neural Networks methods to model interface phenomena in solid phase epitaxy for Silicon
10h40-11h00	*PAUSE café*
11h00-11h30	**O8- F. BRIX**, IJL, Nancy Adsorption energies for atomic oxygen on the Al13Co4(100) surface: a machine learning approach
11h30-12h00	**O9- M. CHAGAS DA SILVA**, LPCT, Nancy Ab initio calculations of finite-temperature properties at multiple electronic structure levels made affordable: An effective combination of perturbation theory and machine learning
12h00-12h30	**Intervention IDRIS -** T. VERY, Orsay – (20 min) **Flash session POSTER** (liste des posters en fin de document)

Buffet et SESSION POSTERS (liste des posters en fin de document)

SESSION 3 – Jeudi 23 septembre après midi

14h00-14h40	**Oratrice invitée : Geneviève DUSSON**, LMB, Besançon An Atomic Cluster Expansion (ACE) to fit interatomic potentials with polynomials
14h40-15h10	**O10- D. BISSUEL** (visio), ILM, Lyon Machine-learned repulsive potentials for the Density Functional based Tight-Binding method
15h10-15h40	*PAUSE café* et SESSION POSTERS (liste des posters en fin de document)
15h40-16h10	**O11- SH. LEE**, CEA-LETI, Grenoble Neural Network Potential for Fast and Accurate Molecular Dynamics Simulations of SiGe
16h10-16h40	**O12- A. CASTELLANO**, CEA-DAM-DIF, Bruyères-Le-Châtel Machine-Learning Assisted Canonical Sampling
16h40-17h10	**O13- P. GRIGOREV**, CINaM, Marseille Synergistic coupling in QM/MM simulations of dislocations via machine learning

SESSION 4 - Vendredi 24 septembre matin

9h-9h40	**Orateur invité : Mihai Cosmin MARINICA**, CEA-SRMP, Gif-sur-Yvette Machine Learning for Atomistic Materials Science
9h40-10h10	**O14- C. LAPOINTE**, CEA-SRMP, Gif-sur-Yvette Modèles de régression de l'entropie vibrationnelle de formation et de migration de défauts ponctuels
10h10–10h30	**O15- TD. SWINBURNE**, CINaM, Marseille Learning how dense dislocation networks evolve
10h30-11h00	*PAUSE café*
11h00-11h30	**O16- AM. GORYAEVA**, CEA-SRMP, Gif-sur-Yvette Reinforcing materials modelling by encoding the structures of defects in crystalline solids into distortion scores
11h30-12h00	**O17- MP. GAIGEOT** (visio), LAMBE, Evry Graph Theory for Molecular Dynamics simulations
12h00-12h30	**O18- G.D. FORSTER** (visio), ICMN, Orléans Approche par deep learning pour déterminer les indices de chiralité des nanotubes de carbone à partir d'images HRTEM

Liste des Présentation Posters

P1. **H. VROYLANDT**, ISCD, Paris
Learning the dynamics of systems with memory: a maximum likelihood approach

P2. **A. FRANCE-LANORD**, ISCD, Paris
Unsupervised learning of atomic-scale dynamics

P3. **JC. CRIVELLO,** ICMPE, Thiais
Supervised learning of DFT results to predict the formation enthalpy of the full set of configurations in complex phases: the sigma-phase as an example

P4. **T. DEVERGNE,** IMPMC, Paris
Machine learning and Umbrella sampling to investigate chemical reactions in solution

P5. **C.A. JARA DONOSO**, LAAS-CNRS, Toulouse
Modeling of Ni-Si interactions through a linearized machine learning potential

P6. **J. HEU**, IMPMC, Paris
Quantum dynamics and Monte Carlo simulations through machine learning

P7. **T. PIGEON**, IFPEN, Lyon
Exploring machine learned collective variables in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions

P8. **B. HERZOG**, LPCT, Nancy
RPA and coupled cluster finite-temperature properties from machine learning thermodynamic perturbation theory

P9. **R. LOT**, LAAS-CNRS, Toulouse – SISSA, Trieste, Italy
PANNA a comprehensive toolkit for creating neural network models for atomistic systems: developer updates

P10. **F. BRIX, E. GAUDRY**, IJL, Nancy
Two-dimensional metal structures revealed by evolutionary computations: Pb/Al13Co4(100) as a case study