Second Edition - Symposium
Artificial Intelligence, machine learning and deep learning approaches in theoretical/ computational chemistry biochemistry, physical-chemistry and material sciences

June 4th 2024
Institut de Chimie Physique, CNRS, Université Paris-Saclay
Salle Magat, building 349, Orsay
https://www.icp.universite-paris-saclay.fr/comment-venir-a-licp/

8h30	Welcome at ICP	
9h	Introduction words	
9h05	Antoine Taly	*Exploring the structure and dynamics of membrane proteins with a combination of AI tools and molecular dynamics*
9h30	Benjamin Bouvier	*Interpreting biomacromolecular structure and dynamics using machine learning*
9h55	Pascal Pernot	*Negative impact of heavy-tailed uncertainty and error distributions on the reliability of calibration statistics for machine learning regression tasks*
10h30	Coffee break	
11h	Markus Meuwly	*Machine Learning Molecular Interactions for Atomistic Simulations*
11h40	Thomas Plé	*FeNNol: an efficient and flexible library for building force-field-enhanced neural networks*
12h05	Lunch - Buffet	
14h	Eric Brémont	*Applying Machine Learning to Save Computational Effort: Chemically-Relevant Examples in Density-Functional Theory*
14h25	Raphaël Vangheluwe & Milica Ritopecki	*Comparison of two machine learning interatomic potentials for metallic nanoparticles*
14h50	Aël Cador	*Hydrolysis barriers in nuclear wastes by molecular simulation and machine learning*
15h15	Coffee break	
15h45	Elise Duboué-Dijon	*Improving the accuracy of QM/MM-MD mechanistic explorations with ML corrections*
16h10	Shoeb Atar	*Data-driven discovery of efficient thermoelectric materials using interpretable machine learning*
16h35	Dounia Zamiati	*Machine Learning-based Clustering of FLIM - Microscopy Data for Automatic Detection of Membrane Contact Sites in Live Cells*
16h45	Conclusions	

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