THEMATIC HALF-DAY AI@UCCS

Reception – Coffee: 13h30

Institut Chevreul, Amphi Chevreul

First Session: Simulation of the Chemistry by Artificial Intelligence

14h00 Nicolas Sisourat (LCPMR, Sorbonne Université, Paris) – Guest Speaker
Speeding-up electronic structure calculation with machine learning

14h40 Jérémie Zaffran (CNRS, Solvay, Chine) – Visio
Computational chemistry, DFT and machine learning to predict heterogenous catalysis

15h00 Egon Heuson - Tao Jiang (UCCS, Centrale Lille, Lille)
Enzyme activity prediction using neural network, docking and high-throughput screening results

15h20 Adlane Sayede (UCCS, Université d'Artois, Lens)
Accelerating the Discovery of New Materials with AI

15h40 Bastien Casier (UCCS, Université d'Artois, Lens)
FCInet: a classification neural network to describe the configuration interaction space

Second Session: Artificial Intelligence in Solide State Chemistry and Catalysis

16h00 Tsveta Miteva (LCPMR, Sorbonne Université, Paris) – Guest Speaker
Artificial intelligence for hyperspectral imaging of historical paintings

16h40 Jorge Benavides (UCCS, Centrale Lille, Lille) – Visio
Artificial intelligence and high-throughput experiments for catalysts design

17h00 Philippe Zinck (UCCS, Université de Lille, Lille)
AI for intricate macromolecular synthesis: from polymer microstructure mapping to inverse polymerization engineering in chain shuttling polymerizations

17h20 Markus Grimm (UCCS, Centrale Lille, Lille)
Towards self-driving labs for heterogeneous catalysis: a Bayesian optimisation approach