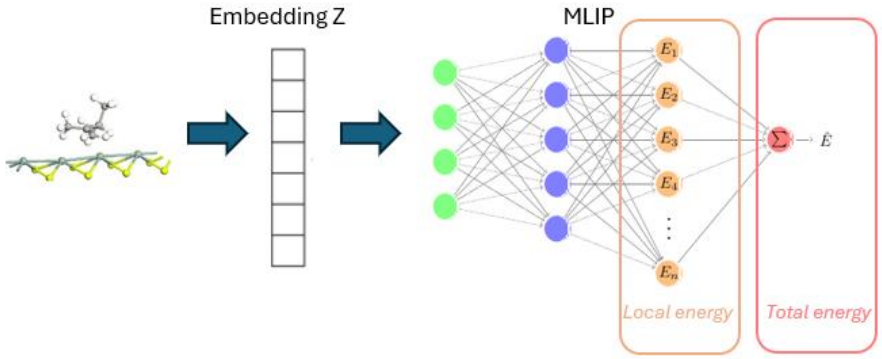
PhD proposal

Quantifying Uncertainty in Machine Learning Interatomic Potentials for Accurate Molecular Dynamics Simulations

In the pursuit of energy transition, optimizing catalytic processes is essential for the efficient and sustainable conversion of raw materials into biofuels. At the heart of this optimization lies a deep understanding of atomic-level reaction mechanisms. However, experimental methods often fall short in accurately identifying active sites and reaction intermediates. Molecular Dynamics (MD) simulations, coupled with quantum mechanical calculations (DFT), provide powerful insights into these mechanisms. Yet, the high computational cost of DFT presents a significant challenge.

To address this limitation, Machine Learning (ML) approaches have emerged as a promising solution, accelerating simulations by replicating DFT results at a fraction of the computational cost using Machine Learning Interatomic Potentials (MLIP). Despite their advantages, MLIP models are prone to accumulating errors during simulations, which can undermine the reliability of the results. Therefore, it is crucial to develop robust methods for real-time error control and estimation to ensure the accuracy of these simulations.



This PhD aims to develop a robust uncertainty quantification framework to control and estimate errors in MLIP-based Molecular Dynamics simulations, enhancing the reliability of reaction rate predictions.

- **Error Control Framework:** Design an uncertainty quantification method that triggers DFT calculations when MLIP errors exceed a predefined threshold**.**
- **Error Propagation in Kinetics:** Develop techniques to propagate uncertainties through MD simulations, enabling accurate estimation of reaction rate constants.
- **Extension to Nonlinear Models:** Adapt the uncertainty quantification framework for nonlinear MLIP models, such as graph neural networks, to broaden its applicability to complex interatomic potentials.

The proposed methods will be validated using the dehydration of isobutanol catalyzed by acidic zeolites—a reaction of significant interest in biomass conversion due to its complexity and industrial relevance. This system serves as an ideal test case to evaluate the accuracy and efficiency of the developed uncertainty quantification framework.

References

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Administrative Details

- Start Date: Fall 2025
- Location: IFPEN, Rueil-Malmaison, France
- Salary: €2,400/month (Year 1) to €2,800/month (Year 3)

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