

Master 2 - Research Training –

Laboratory : PhLAM

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AREA Work Package: WP2

Intitulé du stage et description

Development of force fields using machine learning: the case of actinides

Conventional force fields (MM, traditional force fields) generally provide a satisfactory description of interatomic interactions. However, their ability to represent complex systems, either highly polarizable or with high ion charges, remains limited, such as actinides in solution, but also several processes of atmospheric interest where a detailed description of electrostatic interactions and local electronic response is essential. In our previous work, we developed an advanced classical force field incorporating a large number of physical terms, including n-body contributions, based on ab initio calculations. Despite its accuracy, the parameterization of such a model quickly becomes unfeasible when attempting to include more diverse environments, combining different ligands or counterions, for example.

The objective of this Master's degree is to learn about Machine Learning (ML) approaches in order to design and test a methodology for constructing a new generation of force fields based on Machine Learning (ML) approaches. This model will be trained to accurately reproduce the energy surfaces obtained from ab initio calculations and should enable the precise modeling of the molecular dynamics of the selected systems in their environments.

All of these developments will enable doctoral students to acquire not only solid scientific skills, but also expertise in programming, artificial intelligence, and data processing.

Keywords: Force Field, Artificial Intelligence, Molecular Dynamics, Actinides