

## Contrats doctoraux 2026

**Titre du projet de thèse :** Development of force fields using machine learning: the case of actinides

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### Résumé du projet de thèse (en 20 lignes maximum) :

Classical force fields (MM, traditional force fields) generally provide a satisfactory description of interatomic interactions. However, their ability to represent complex systems—whether highly polarizable or with high ionic charges—remains limited, such as actinides in solution, as well as several processes of atmospheric interest where a detailed description of electrostatic interactions and the 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, and based on ab initio calculations. Despite its accuracy, the parameterization of such a model quickly becomes unfeasible as soon as one wishes to include more diverse environments, combining different ligands or counterions, for example.

The objective of this thesis is to design and test a methodology for constructing a next-generation force field based on machine learning (ML) approaches. This model will be trained to faithfully reproduce the energy surfaces derived from ab initio calculations and should enable the accurate modeling of the molecular dynamics of selected systems in their environments. Such an ML force field will offer greater flexibility compared to traditional parameterized approaches, allowing for the natural integration of complex and nonlinear interactions, while maintaining accuracy close to that of ab initio methods and significantly reducing computational costs.

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

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**Remarques/commentaires supplémentaires :**

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