Internship advertisement

Université Paris Saclay

Predicting thermodynamic properties of defects in medium-entropy alloys from the atomic scale through statistical learning

Understanding the behaviour of materials under extreme conditions is essential for the design of future energy systems, such as fission and fusion reactors. However, accurately predicting the properties of materials at high temperatures remains a challenge. Direct measurements of these properties are limited by experimental instrumentation, and atomic-scale simulations based on empirical force fields are often unreliable due to a lack of precision. This problem can be solved using statistical learning techniques, which have recently seen their use explode in materials science. Force fields constructed by statistical learning achieve the degree of accuracy of *ab initio* calculations ; however, their implementation in sampling methods is limited by high computational costs, generally several orders of magnitude higher than those of traditional force fields. To overcome this limitation, two avenues have traditionally been explored : (i) improving active statistical learning force fields by finding a better accuracy-efficiency trade-off and (ii) creating accelerated free energy and kinetic path sampling methods to facilitate the use of computationally expensive statistical learning force fields.

During this internship, we will focus on the descriptor of the local atomic environment and the regression model. We will then implement a fast and robust Bayesian sampling scheme to estimate the free energy, an essential thermodynamic quantity that allows us to understand the effects of temperature in crystalline solids and that provides, among other things, access to the thermodynamic properties of point defects. The aim here will be to estimate the free energies of formation and migration of vacancy defects, which, using kinetic Monte Carlo simulations, make it possible to estimate the atomic diffusion coefficients in complex alloys. Specifically, we will use an algorithmic extension to restrict Bayesian sampling to a specific metastable basin or to transition paths connecting two adjacent metastable basins. The study will focus on a complex alloy to be defined comprising the elements W, Ti, V, Mo and Ta.

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This six-month internship may be followed by a thesis under a doctoral contract with CEA.

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