12 months post-doctoral position available

Sensitivity analysis and learning techniques for mapping the thermodynamic properties of alloys.

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The determination and understanding of bulk phase diagrams is a prerequisite for the study of more complex phase diagrams, such as those of alloy surfaces or nano-alloys. Current calculations are mainly based on cluster expansion (CE), which allows the determination of interaction energies. The phase diagram is then obtained by statistical lattice physics methods (CVM or Monte Carlo simulations). While these approaches are very powerful for systems with low parametric mismatch between the two constituents, they are limited for systems with high parametric mismatch, for which the role of atomic relaxations is important. Optimization coupling structural relaxations and constituent distribution is still a blocking point in materials modeling. Simulations with semi-empirical interatomic potentials make it possible to overcome this issue. It is possible to determine the equilibrium properties of the system using Monte Carlo simulations that allow the optimization of both the atomic positions and the chemical distribution of the constituents. However, these simulations do not permit distinguishing chemical effects (due to short-range interactions) from long-range effects (due to the size difference between the constituents). Moreover, there are no direct links between the parameters of the potentials and the phase diagrams, so it is a priori impossible to predict the thermodynamic properties of the alloys from the interatomic potentials.

Recently we have developed a method[1] for the determination and analysis of phase diagrams. This method, based on the use of interatomic potentials, paves the way for the elaboration of a mapping of the thermodynamic properties of alloys, which has never been done before. However, the process of characterizing the thermodynamic properties can quickly become time-consuming. The use of powerful techniques can reduce this problem by limiting the exploration domain to the discriminant parameters (which have a strong influence on the model outputs) identified through sensitivity analysis[2]. Machine learning (ML) will allow investigating the discriminant parameters efficiently and predicting quickly the properties of the model.

The hired postdoctoral fellow will be in charge of the local sensitivity analysis[3]. It consists in developing the formalism under small variation assumptions using appropriate Taylor series developments to account for uncertainties. We will first consider alloys previously studied in the team to test the validity of these developments. The post-doctoral fellow will have to develop the screening method using random procedures. Sensitivity analysis will be used to reduce the number of model parameters. Once the inputs and outputs are simplified, the objective is to verify whether it is possible to replace direct numerical simulation by a metamodel[4] to establish behavioural maps of the thermodynamic properties of alloys.

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[1] F. Berthier et al., Phys. Rev. B 95, 224102 (2017) ; F. Berthier et al., Phys. Rev. B 99, 014108 (2019).
[2] A. Saltelli et al., Sensitivity Analysis, John Whiley & Sons (2006).
[3] N. Carrasco *et al.*, *Planet. Space Sci.* 55, 1644–1657 (2008); M. Dobrijevic *et al.*, *Planet. Space Sci.* 56, 1630–1643 (2008).
[4] F. Cailliez and P. Pernot, *J. Chem. Phys.* 134, 054124 (2011); F. Cailliez *et al.*, *J. Comput. Chem.* 35, 130–149 (2013)

Qualifications : The successful candidate will must have earned a PhD degree in Solid State Physics, Materials Science or in a closely related area. Good English language proficiency. Ideal candidates will have a few years of experience in atomic scale simulation. Programming experience, e. g. in python, are advantageous. The candidate needs to be highly motivated and capable of performing research in an autonomous and rigorous way.

Pratical information : The post-doctoral fellow will be posted at the ICMMO in the Université Paris-Saclay. The laboratory is located 20 km south-west of Paris, it is connected by public transportation.

Time frame : The position is funded for 12 months and it will possibly start in October 2020.

How to apply : Candidates should send their application (coverletter, CV with list of publications and contact information of two references) to Fabienne Berthier (fabienne.berthier@universite-paris-saclay.fr),

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