Postdoctoral position

Atomistic simulations and active learning to predict thermodynamic properties in a large chemical space

Duration: 1 year starting from October to December 2023

Location: SIMaP laboratory, "Thermodynamics, Modelling and Process Optimisation" group, Grenoble, France

Contact: Guillaume DEFFRENNES, CNRS research associate, at guillaume.deffrennes@cnrs.fr

Context

The enthalpy of mixing is an important property to predict phase equilibria through machine learning[1] or thermodynamic calculations[2]. Currently, only a semi-empirical model[3] developed in 1980 allows to easily estimate this property, and it is only applicable to the liquid phase. We are working on developing machine learning models to predict the enthalpy of mixing in liquid and solid solutions for all binary combinations of 60 elements. To that end, experimental data have been collected. New training data can be obtained from atomistic simulations, but only a fraction of the possible compositions can be covered.

Main duties

As a postdoctoral fellow funded by the MIAI Grenoble Alpes institute (https://miai.univ-grenoble-alpes.fr), you will contribute to this project by:

- generating high-quality data using molecular dynamics simulations (for the liquid phase) and the special quasi-random structures method (for solid solutions)
- developing an active learning strategy to identify the most informative simulations, i.e., where in the chemical space new data are most needed
- creating automated data collection workflows

You will work with collaborators in France and in Japan.

Candidate profile

We are looking for highly motivated candidates with:

- a PhD in materials science, physics or chemistry
- a background in atomistic simulations
- an interest in machine learning, thermodynamics, computational science and coding

How to apply: please send a CV, up to two publications, and at least one reference we can contact for a recommendation to guillaume.deffrennes@cnrs.fr. Applicants are encouraged to apply as soon as possible, and before the end of September.

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[1] Deffrennes *et al.*, Materials & Design 232 (2023), https://doi.org/10.1016/j.matdes.2023.112111
[2] Chen *et al.*, Nature Communications 14 (2023), https://doi.org/10.1038/s41467-023-38423-7
[3] Miedema *et al.*, Physica B+C 100 (1980), https://doi.org/10.1016/0378-4363(80)90054-6