SIMaP
Science et Ingénierie
des Matériaux et des Procédés

Bio-Inspired Global Optimization for Multicomponent Nanoalloys

SIMaP, Saint-Martin-d'Hères, France
6 months M2 Internship

Research context

Predicting the most stable atomic structures of metallic nanoparticles and nanoalloys is a challenging computational problem due to the large number of possible atomic configurations and chemical arrangements. As the number of chemical elements increases, exploring the corresponding potential energy landscape becomes increasingly complex.

The objective of this internship is to benchmark bio-inspired global optimization algorithms for predicting stable structures of multicomponent metallic nanoparticles containing up to five chemical elements. The project combines computational materials science, numerical optimization, and scientific programming, with a particular focus on comparing the efficiency, reliability, and computational cost of different optimization strategies.This internship was approved and will be funded by the DIADEM Master Project program 2026/2027.

Internship objectives and activities

The selected candidate will contribute to the /development of a Python-based computational framework for nanoparticle structure optimization.
The main activities will include:

- **Scientific programming:** Develop a common optimization framework using Python and the Atomic Simulation Environment (ASE).
- **Bio-inspired optimization:** Implement and evaluate Genetic Algorithms (GA), Differential Evolution (DE), and Particle Swarm Optimization (PSO).
- **Atomistic simulations:** Perform energy calculations and structural relaxation using LAMMPS and interatomic potentials using ASE, with possible extensions to xTB.
- **Algorithm benchmarking:** Compare bio-inspired methods against conventional approaches, including Basin Hopping and Minima Hopping.
- **Performance analysis:** Investigate convergence, computational efficiency, structural diversity, and the influence of chemical complexity.
- **High-performance computing (HPC):** Run computational experiments on HPC infrastructure, particularly GRICAD.

The internship will result in a reusable computational framework and a comparative analysis of optimization methods for multicomponent nanoalloys.

Candidate profile

We welcome applications from M2 students in Physics, Computational Materials Science, Applied Mathematics, Computer Science, Computational Chemistry, or related fields.

Required skills:

- Demonstrated programming skills in Python.
- Basic knowledge of numerical methods, optimization, or computational physics.
- Interest in scientific computing and algorithm development.
- Ability to work independently and analyze numerical results.

Additional skills appreciated (not mandatory):

- Experience with atomistic simulations, molecular dynamics, or materials modeling.
- Familiarity with ASE, LAMMPS, NumPy, SciPy, or optimization libraries (pymoo, DEAP).
- Knowledge of evolutionary algorithms, metaheuristics, or machine learning.
- Experience with Linux environments, parallel computing, or HPC clusters.

Prior experience with all the mentioned software packages is **not required**. The internship provides opportunities to develop expertise in global optimization, atomistic simulations, and high-performance scientific computing.

Some additional RH information

The approximate internship stipend is **€685 per month** (this is not a salary). **The internship will begin no earlier than early February**. Since the internship stipend will be paid by the CNRS through the PEPR, a request for access must be submitted to the FSD, for the selected candidate, regardless of their nationality. This process requires a processing/response time of 2 months.

Application and contact

Interested candidates are invited to send a **CV and a short motivation letter**, highlighting their programming experience and interest in the project.

For applications or further information, please contact:

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