

Master thesis proposal

Melting Point Simulation of Bi-Pt Nanoparticles for Miniaturized Thermal Sensors Using AI (ChiMES/MACE + Fine-Tuning)

Keywords : Nanoparticles, Bi-Pt, Melting point, Molecular dynamics, Machine learning potentials (MACE, ChiMES), DFT, Thermal sensors, AI for materials

SCIENTIFIC DESCRIPTION :

The precise control of the melting point of metallic nanoparticles is essential for applications in catalysis, conductive inks, and miniaturized thermal sensors. Conventional temperature probes often fail under extreme conditions, while bimetallic nanoparticles such as bismuth-platinum (Bi-Pt) offer a promising alternative thanks to their tunable thermal properties.

In this project, the student will exploit machine learning potentials (ChiMES, MACE), trained on density functional theory (DFT) data, to perform molecular dynamics simulations at variable temperatures. The goal is to determine how size, morphology, and composition affect the melting point of Bi-Pt nanoparticles. Fine-tuning strategies on complementary DFT calculations will be implemented to improve model accuracy. The results will provide methodological tools for the rational design of nanomaterials for thermal sensing, with direct connections to ongoing projects on conductive inks (Ag-Cu systems, COCAPEC).

Techniques/methods in use :

- Atomistic simulations (DFT, molecular dynamics)
- Machine learning interatomic potentials (MACE, ChiMES)
- Structure optimization (Particle Swarm Optimization)
- Data-driven model fine-tuning and uncertainty quantification

Applicant skills : Background in physics, chemistry, or materials science; basic programming (Python preferred); interest in artificial intelligence applied to materials modeling.

Industrial partnership : SATT Paris-Saclay (COCAPEC project – Ag-Cu conductive inks).

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Possibility for a Doctoral thesis : Yes

