The Nanoscience Cooperative Research Center, CIC nanoGUNE, located in Donostia / San Sebastian, Basque Country (Spain), is currently looking for a

MASTER STUDENT

to work on

Towards machine learning models for the potential energy surface with accurate stability of crystal polymorphs

NanoGUNE is a research center devoted to conducting world-class nanoscience research for a competitive growth of the Basque Country. NanoGUNE is a member of the Basque Research and Technology Alliance (BRTA) and is recognized by the Spanish Research Agency as a *María de Maeztu* Unit of Excellence.

The **position** is offered in the Theory Group. More information can be found at: https://www.nanogune.eu/en/research/groups/theory

Project Director: **Pablo Piaggi** (pm.piaggi@nanogune.eu)

Project Description

Atomistic simulations have become an essential technique in condensed-matter physics and materials science, complementing experiments and giving access to a broad range of properties, including phase diagrams and crystal polymorph stability. The results of such simulations depend crucially on the model for the potential energy surface (PES), which is used to derive the interatomic forces that drive the dynamics. The advent of artificial intelligence has completely changed the landscape of this field and currently machine learning models for the PES are used routinely to simulate materials with unprecedented accuracy and efficiency. Such models are trained on quantum-mechanical density-functional theory (ab initio) calculations, and approximations in these calculations often give rise to a deviation of the predicted properties with respect to experiment. The thermodynamic stability of crystal polymorphs is a sensitive test of the quality of the PES, and melting and coexistence lines often show differences of more than 10% with respect to experiment. In this project, we will apply an algorithm recently developed in my team [Peña-Cano and Piaggi, arXiv:2511.14352 (2025)] aimed at generating machine learning models for the PES that combine ab initio and experimental data. This approach will be applied to the training of a model for a system with at least two crystal polymorphs, and we will seek to create a model that accurately reproduces the phase diagram for such a substance. In this way, we aim to construct a machine-learning model for the PES that ranks among the most accurate and advanced available for molecular dynamics to date..

Candidates should **apply** by following the instructions and reccomendations of the general call and by completing the form below and attaching the following documents:

a. A complete CV
b. Academic record and cover letter grouped in a single PDF file

The **deadline** for applications is **06/04/2026**.

NOTES:
(i) All applicants will receive an answer after the end of the selection process; but please note that due to the large number of submissions that are expected, we cannot provide individual feedback.

(ii) Additional information about nanoGUNE's commitment towards HR excellence in Research and Gender Equality are available on our website.
(iii) We encourage you to subscribe to our HR mailing list to receive information related to nanoGUNE's open positions and open calls for different training and talent attraction programs.