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

Deep learning for simulating crystal nucleation

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.

Crystal nucleation, the initial phase in the formation of crystalline solids, is notoriously difficult to observe within the time scales accessible to standard molecular simulations. A successful route to overcoming this challenge is the use of enhanced sampling methods based on the introduction of a bias potential which is a function of a small number of collective variables. The determination of collective variables was typically a difficult endeavor and often relied on physical intuition. In the last five years, the advent of deep learning (machine learning with deep neural networks) has started to provide new tools for systematically deriving optimal collective variables.

In this **project**, we will adapt recent advances in this field, including graph neural networks, to the study of crystal nucleation. This task requires training machine-learned collective variables suitable to study these processes, applying them to perform biased simulations, computing nucleation free energy barriers, and obtaining microscopic insight into crystal nucleation processes. We envisage an initial application to a simple case, such as the nucleation of metals from the melt, and later tackling the challenging case of crystal nucleation from solution. The ultimate goal of this project is leveraging deep learning to develop a general and systematic framework to tackle crystal nucleation in molecular simulations.

Supervisor: **Pablo M. Piaggi** (pm.piaggi@nanogune.eu)

Candidates should **apply** by completing the **form below** and attaching the following documents:

a. A complete CV

b. A cover letter

The **deadline** for applications is **13/03/2025**.

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.