

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.

The aim of the research **project** is 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. The student will be supervised by **Pablo Piaggi** (pm.piaggi@nanogune.eu).

The position is offered in the **Theory Group**, led by **Emilio Artacho** (e.artacho@nanogune.eu). More information can be found at <https://www.nanogune.eu/en/research>.

The position is expected to start in **01/09/2025** and for a total length of up to **10 months** (01/09/2025 - 30/06/2026).

Candidates should **apply** 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 **22/06/2025**.

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.