

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

Exploring topological chemical space through quantum algorithms

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**, led by Emilio Artacho. More information can be found at <https://www.nanogune.eu/en/research/groups/theory>

Project Description

Quantum computing offers a new paradigm for solving electronic structure problems, which are central to quantum chemistry, condensed matter physics, and materials science. This is especially relevant whenever classical methods such as density functional theory or exact diagonalization face increasing or even prohibitive computational cost. In this regard, quantum algorithms provide a promising alternative by using quantum circuits to efficiently represent (many-body) electronic wavefunctions. Motivated by recent experimental realization of half-Möbius electronic topology in a single molecule, this project seeks to move beyond trivial benchmarks of simple molecules in order to explore the "molecular topological space". Using a range of quantum algorithms and on-going inhouse theoretical development, we will conduct a systematic search for new families of molecules with non-trivial electronic phases. Such topological molecular design holds the potential to unlock entirely new classes of materials for quantum sensing, with the chemical behavior dictated by the geometry of the wavefunction itself. This project develops original methods at the intersection of quantum algorithms and topological chemistry, providing a strong foundation in both quantum computing and modern electronic structure theory. The master work can be continued as a Ph.D.

Project Director: **Daniel Hernangómez Pérez** (d.hernangomez@nanogune.eu)

Candidates should **apply** by following the instructions and recommendations 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.*

