

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
MINECO_RETOS_2019_FunMolSys_CIC07_Pascual-Artacho

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 Artacho Cortés, Emilio (e.artacho@nanogune.eu). The Theory Research Group works both in the development of simulation techniques and in their application to different problems..

The candidate will join a **research line** focusing on Computational and theoretical condensed matter physics. Complex solids and liquids, using first-principles molecular dynamics based on density-functional theory and on linear-scaling density-functional theory. Nanoscale oxide heterostructures including multiferroics, liquid water, and water/solid interfaces, and non-adiabatic processes related to radiation damage of materials.. More information can be found at <https://www.nanogune.eu/theory>.

The aim of the **project** is to - Project: CIC072019001 - Magnetismo y estados topológicos de sistemas moleculares creados en superficies -FunMolSys

- Introduction: SHORT DESCRIPTION: Water confined to nanometric dimensions changes its properties in various ways. This is very relevant for understanding the behaviour of water when confined between macromolecules and organelles in a living cell, for instance. After characterizing the structure and phases of water confined to ultrathin sheets, we propose to study the flow characteristics of that liquid, which should be very different to that of bulk water and of conventional fluids.

- Work Plan: DETAILS OF THE PROJECT: The project will consist of simulations of the motion of water molecules (molecular dynamics simulations) conforming the liquid, as confined by flat walls, and under flow conditions. The analysis of how these molecules move depending on how they interact with other molecules and to the confining walls, will show the kind of flow, and how to alter and tailor it.

DESCRIPTION OF THE GROUP: The Theory group of Nanogune has ample experience in the description of condensed matter from first-principles simulations, in general, and molecular dynamics, in particular, including very thorough studies of liquid water, both in bulk and in nanoconfined conditions.

TASKS: Different simulations will be established and performed for water films of different thicknesses, and different average flow, for simulation cells with enough number of molecules, and for time scales long enough to allow defining stationary flow.

OBJECTIVES: Obtain the velocity profile across the confined direction(s) as a function of position. Extract differences due to alterations to the confining surface, namely, the attractive interaction and the roughness.

WORK MATERIALS: The work is theoretical and computational, and will involve the use of supercomputers using parallel computing. The programs will be provided.

START DATE: Whatever appropriate for a TFM

END DATE: Whatever appropriate for a TFM

TIMETABLE: Flexible

TOTAL NUMBER OF HOURS: Whatever appropriate for a TFM
LANGUAGE: English.

The successful **candidate** will have a .
Additionally, the candidate should demonstrate experience in the following skills:
Although not compulsory, the following points will be considered:

- **We promote** teamwork in a diverse and inclusive environment and welcome all kinds of applicants regardless of age, disability, gender, nationality, race, religion, or sexual orientation.

The position is expected to start in 01/10/2021 and for a total length of up to 10 months (01/10/2021 - 31/07/2022) in the Theory Group. The contract will be funded by the .

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

- a. A complete CV
- b. A cover letter and at least two reference letters grouped in a single PDF file

The **deadline** for applications is **30/06/2021**.

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.