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.

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 research 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. For more information, see our website at https://www.nanogune.eu/en/research/groups/theory

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.

Application:

If you are a master student and you are interested in this project, please get in touch with the scientist in charge: **Emilio Artacho** (e.artacho@nanogune.eu).

To apply for a **master position** fill in the form below and follow the instructions and recommendations of the general call (**open until 31 July 2023**).

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.