

Domain wall engineering is the technique consisting in exploiting the properties of domain walls in ferroic materials for applications, as opposed to using the properties of the bulk of the material. In ferroelectric materials, domain walls display a number of properties that are of great interest for practical applications, such as electrical conductivity (in an otherwise insulating material), negative capacitance or chirality. Using computational simulations we can study these systems and learn how to best harness their properties.

Details of the project:

Using a combination of programs capable of describing quantum electronic processes in condensed matter and phenomenological models, the project aims to characterize charged domain walls in ferroelectric material using computer simulations.

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 in the study of ferroelectric materials, in particular. For more information, see our website at <https://www.nanogune.eu/en/research/groups/theory>

Tasks:

Perform a series of atomistic simulations of a ferroelectric material under various boundary and doping conditions. Extract information from the quantum-mechanical simulations and develop a phenomenological model to predict the properties of charged domain walls in the system. This information will then be used for the design of large scale simulations of domain walls.

Objectives:

Understand the physics of charged domain walls in ferroelectric materials and be able to predict from the models the conditions that may produce domain walls with the desired properties.

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: **Pablo Aguado Puente** (p.aguado@nanogune.eu).

To apply for a master scholarship fill in the form below and follow the instructions and recommendations of the general call (**open until 30 June 2022**).

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.