The recent study [AW Kuziel, et al., Adv. Mater. 32, 2000608 (2020)] into graphene flakes has shown that small pristine flakes are 2D amphiphiles that can be a versatile 2D stabiliser ideal for a broad range of environmental, geological, or biomedical technologies. Rigorous quantum-mechanical, molecular dynamics and Monte Carlo calculations supported by experiments have revealed that pristine graphene flakes with the small surface areas can form ultrastable water/oil emulsions due to well-defined hydrophobic and hydrophilic regions in the basal plane and edges, respectively. Their amphipathic strength can be controlled by varying the flake size and its thickness. The interactions between flakes can be also controlled by varying the oil-to-water ratio. Small and thin pristine graphene flakes can be efficiently used under high pressure, combined with high temperatures and in saline solutions overcoming many of the limitations of current surfactants.

The aim of the Master project is to investigate the chemical nature of other stable 2D materials flakes and their interactions with solvents by means of density functional theory (DFT) combined with molecular dynamic (MD) 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 simulation of radiation damage, in particular. For more information, see our website at https://www.nanogune.eu/en/research/groups/theory

Tasks:

1. Establish, perform and analyse a series of DFT calculations of solvent-flakes systems to understand the interactions between solvent molecules and chosen nanoplatelets.
2. Establish, perform and analyse a series of MD simulations of the most promising 2D flakes in oil-water mixtures to study their emulsifying character.

Objectives:

Understand the chemical nature of selected 2D materials and identify the most promising stabilizers.

Work materials:

The work is theoretical and computational, and will involve parallel computing on computational clusters. Numerical packages necessary to perform all simulations 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: **Karolina Zofia Milowska** (kz.milowska@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.