CIC nanoGUNE
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

Description of the project:

Emulsification of low-dimensional materials is an effective method for formation of macroscopic structures while preserving the degree of particle exfoliation, facilitating the formation of 3D self-assembled structures with novel properties.

Solid emulsifiers have several advantages over the typical surfactants. Pickering emulsions are extremely stable and are not susceptible to spontaneous phase separation. Some of 2D materials can also stabilize oil-water emulsions.

Emulsification of low-dimensional materials is an effective method for formation of macroscopic structures while preserving the degree of particle exfoliation, facilitating the formation of 3D self-assembled structures with novel properties. Solid emulsifiers have several advantages over the typical surfactants that are among the most prominent contaminants continuously released into the environment [1]. Such emulsions, reported for the first time in 1907 by Pickering, display a high resistance to coalescence (and hence de-emulsification) over time and under elevated temperature accompanied by the optional recovery of the solids. The Pickering emulsions employs solid nano- to micro-sized particles localized at the oil-water interface in place of the surfactants. Many materials of sizes in the range from few nanometres to few micrometers exhibit distinctive properties unseen in their smaller as well as larger counterparts or in the bulk. Some of 2D materials commonly considered as hydrophobic in their bigger forms can stabilize water-oil emulsions [2,3]. In particular, it is possible not only to use graphene derivative, such as graphene oxide (GO) [4], but also pristine graphene flakes (GF) to prepare ultra-stable emulsions [5]. Well-defined hydrophobic basal plane and hydrophilic edges of small and thin GF enable them to be used as alternative surfactants for a broad range of environmental, geological, or biomedical technologies. GO, G, as well as hBN, MoS2 and WS2 can equip the emulsions with added value properties such as an increased electro- and thermoconductivity, stimuli-responsiveness and/or porosity under certain conditions. However, besides G and GO, the physico-chemical mechanism behind this behaviour is unknown.

The aim of the Master project is to investigate the chemical nature of transition metal flakes and their interactions with solvents by means of density functional theory (DFT) combined with molecular dynamic (MD) simulations.

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 in the simulation of radiation damage, in particular.

Objectives:

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

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.

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.

- Start date: Whatever appropiate for TFM
- End date: Whatever appropiate for TFM
- Timetable: Flexible
- Total number of hours: Whatever appropiate for TFM
- Language: English

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 position** fill in the form below and follow the instructions and recommendations of the general call (**open until 30 June 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.