CIC nanoGUNE
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

Description of the project:

Reaching structural homogeneity in nanomaterials is crucial for drawing meaningful conclusions about their nature. Various purification methods have been developed to solve this issue, but their utility is hampered by the limited understanding of the underlying phenomena.

With their auspicious characteristics, single-walled carbon nanotubes (SWCNTs) remain at the forefront of research despite being discovered 30 years ago. Unfortunately, several technological constraints still hamper their implementation in real life. One of the grand challenges, which remains unresolved, is the scarcity of appropriate methods to control the structure of SWCNTs at the atomic level. An arsenal of SWCNT differentiation methods has been developed to tackle this problem. Among them, conjugated polymer extraction (CPE) is promising as it enables the isolation of chirality-enriched SWCNTs in organic solvents, which can be directly deposited on substrates to make devices. Unfortunately, despite a plethora of articles on this topic, only two protocols were established over a decade ago that can provide monochiral SWCNT fractions, i.e. (6,5), and (7,5), using PFO-BPy and PFO polymers, respectively. The extension of the spectrum of available chiralities is currently not possible as the mechanism of CPE has not been elucidated due to the price-prohibitive character of the polymers used for the extraction. Consequently, the community has not been able to conduct a sufficiently deep analysis to obtain the necessary insight.

The aim of the Master project is to find new conjugated polymers that will enable efficient sorting of small semiconducting nanotubes by means of molecular dynamic (MD) and time-step force-bias Monte Carlo (MC) simulations combined with density functional tight binding method (DFTB) calculations with close collaboration with experimental group.

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 the interactions between small semiconducting carbon nanotubes and chosen conjugated polymers and identify the most promising sorting agents.

Tasks:

1. Establish, perform and analyse a series of MD/MC simulations of chosen conjugated polymers and carbon nanotubes suspended in chosen solvent systems to understand the interactions between all three components of the system.
2. Establish, perform and analyse DFTB simulations of the representative screenshots from MD/MC simulations to fully understand the CPE mechanism.

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.