

OFERTA DE PROYECTO DE TESIS DOCTORAL, AYUDAS PARA LA FORMACIÓN DE PROFESORADO UNIVERSITARIO (FPU 2019)

Información General

Área de Investigación
Centro/Instituto
Grupo de Investigación
Tema de investigación del grupo:
Provincia
Correo de contacto
Página Web de referencia

Detalles Sobre la Oferta

Referencia proyecto
Tema de Investigación:
Ámbito (dentro del área de investigación):
Palabras Clave



Resumen del Proyecto (100-3000 palabras)

In the last years two-dimensional (2D) materials have emerged as a new family of building blocks for membranes which are expected to achieve low transport resistance as well as high selectivity. Among them we highlight graphene and hexagonal boron nitride (h-BN) which have been recently reported (experiments from the group of Geim in Manchester (UK)) to allow proton or hydrogen conduction with low energy barriers, opening the possibility to use them as efficient proton transfer membranes or hydrogen isotope separation medium. However, how protons or hydrogens conduct across or along the 2D crystal is still unclear since recent theoretically predictions do not fully agree with the experimental findings.

The aim of this project is to theoretically provide a reliable interpretation of the above mentioned experimental results by means of density functional theory (DFT) and density functional tight binding (DFTB) approaches. In particular, the use of molecular prototypes to describe the membranes based on graphene and h-BN is first proposed and the possibility of their protonation/hydrogenation will be carefully investigated. Then, the different mechanisms capable to efficiently produce the proton /hydrogen permeation and diffusion across and along the 2D plane will be studied and assessed. The project will also take into account the role of the solvent, as well as that of the use of periodic models to describe the 2D membranes.