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

Información General

Área de Investigación
Física y Tecnologías Físicas
Centro/Instituto
Instituto de Física Fundamental
Grupo de Investigación
INTERMOL
Tema de investigación del grupo:
Teoria y simulación de interacciones moleculares y materiales 2d
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Detalles Sobre la Oferta

Referencia proyecto
Tema de Investigación:
Almacenamiento de hidrógeno en materiales 2D nanoporosos
Ámbito (dentro del área de investigación):
Materiales nanoporosos, energía, almacenamiento hidrógeno
Palabras Clave
Materiales 2D, almacenamiento de hidrógeno, simulación computacional

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Resumen del Proyecto (100-3000 palabras)

The quest for clean, safe and affordable sources of energies has spurred research in many directions and one of the most promising combustible species that has been found is hydrogen since its combustion generates only water, releasing at the same time a great amount of energy. Hydrogen is the lightest molecule and the storage and release of this new generation of fuels is a key step in developing an attractive industrial manufactured product for a sustainable and green society[1].

Traditional storage devices including high pressure deposit, or liquid transport and storage are not suitable for individual or community uses and it might not be adequate even in large storage production and conversion facilities. To avoid these problems the use of porous materials has been presented as an efficient alternative because of the high specific surface that helps increasing the gravimetric capacity. We think that porous carbon materials are worth to explore as one of these candidates for hydrogen storage at a room temperature. Since the the binding of hydrogen molecules to these porous or nanoporous substrates is ruled by weak intermolecular forces, the management of transport and refilling operations will be simple and safe. However, these interactions should be somehow stronger in order to increase the gravimetric capacity. Doping of carbon materials with alkali and alkali-earth metal has been proposed as a mean to enhance the adsorption energy while stabilizing the substrate against destruction during adsorption/desorption process[2].

We propose to study the adsorption of hydrogen on ion-doped carbon materials as a reliable alternative for hydrogen storage. Our group has already experience in dealing with nanoporous materials [3-5], and is collaborating with other groups in the study of large clusters involving H2 with Li+, and Cs + [6]. The project includes the computation of adequate interaction potential energy surface, and classical and quantum Monte Carlo techniques for the adsorption problem. The dynamical processes and the proposition of nanoporous carbon materials will be dealt with molecular dynamics simulations with a special emphasis in the possible influence of quantum effects for what we will rely on quantum wave packet techniques and transition state theory[4].

References:

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[5] M. I. Hernández et al., J. Phys. Chem. A, 119, 10743 (2015).
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