Theoretical simulations of novel Magnetic Carbides immersed in a graphene-based matrix

Investigadores:

- César González. Universidad Complutense de Madrid (UCM [1]).

Idioma Sin definir

Descripción:
Proyecto asignado a través de la Red Española de Supercomputación (RES [2]).

Motivated by the recent synthesis of magnetic carbides nanoparticles (NP) developed at the Institute of Applied Magnetism, we propose the theoretical study, based on the Density Functional Theory (DFT), of the interface formed between the iron carbide, the so-called cementite (Fe3C) with a graphitic layer that covers the NP. The determination of the interaction established between both subsystems is of paramount importance for the understanding of the magnetic properties of the NPs and their further application as efficient lightweight microwave absorbing material. The theoretical calculations can help in the atomic and magnetic characterization of such complex interface as well as the most favorable Fe3C surface for the graphite adsorption. The large unit cells required by the simulations demands the use of supercomputer facilities.

URL del envío:https://www.cenits.es/proyectos/theoretical-simulations-novel-magnetic-carbides-immersed-graphene-based-matrix

Enlaces
[1] https://www.ucm.es/ [2] https://www.res.es/