

## DFT simulations on the study of the dielectric function of novel nanostructured materials

## Researchers:

• Francesca Peiró. Universitat de Barcelona.

Language Undefined

## **Description:**

Proyecto asignado a través de la Red Española de Supercomputación (RES [1]).

In the present work, the anisotropic electrical conductivity of GalnP CuPtB type ordered layers will be assessed by using in-situ biasing in a Transmission Electron Microscopy (TEM). The electrical conductivity of GalnP thin films with different degree of order (controlled by the amount of Sb flux during the growth) will be measured in the orthogonal [110] and [1-10] directions. The anisotropy will be evaluated as a function of the density of ordered domains and antiphase boundaries and the results will be discussed in the light of DFT simulations.

Web:

Source URL: https://www.cenits.es/en/proyectos/dft-simulations-study-dielectric-function-novel-nanostructured-materials

## Links

[1] https://www.res.es/