Predicting thermoelastic properties of 2D materials

Researchers:

- Jose Javier Plata Ramos. Universidad de Sevilla [1].

Language Undefined

Description:

Proyecto asignado a través de la Red Española de Supercomputación [2].

Since the isolation of graphene, two dimensional (2D) materials have attracted the attention due to their exceptional and exotic mechanical, electronic, thermal, and optical properties for potential applications in different key technologies. The prediction of most of their electronic and mechanical properties using DFT commercial packages is considered as routine. However, static DFT calculations does not include thermal effects, so the prediction of materials properties such as elasticity on working conditions and their thermal stability remains as a challenge. In previous periods, we established a new methodology to predict the thermoelastic properties of ultra-high temperature ceramics, reducing the computational cost. In this activity, we strive to calculate the temperature-dependent elastic constants of 2D materials.

Links

[1] https://www.us.es/ [2] https://www.res.es/