Title:

Two-dimensional materials for energy conversion and storage: Computational predictions of physical properties using Density Functional Theory (DFT)

Abdelilah Benyoussef

Hassan II Academy of Sciences and Technology, Rabat, Morocco

LaMCScI, Faculty of Sciences, Mohammed V University, Rabat, Morocco

Abstract:

The discovery of two-dimensional materials has created a new era of materials science with applications in energy and spintronics. New thin-film materials, mechanically, thermally and electronically stable, are available and used for the manufacture of ultra-thin flexible devices. Understanding the properties of two-dimensional materials is based on electronic properties. The functional density theory is a powerful method of quantum mechanics for the design of two-dimensional materials. It does not use parameters derived experimentally, the crystalline structure of the material is the only entry in these DFT calculations, but even this structure can also be calculated by the DFT. Phosphorene, a two-dimensional analogue of graphene, has recently been discovered. It is suitable as a photocatalyst for the production of hydrogen. In addition, it is a promising anode material for ion batteries (Li / Na / Mg). Solid state hydrogen storage is based on the interaction between hydrogen and the surface of the storage material. The storage capacities of nanostructured materials are high because of their enormous surface area. Phosphorene is a promising material for storing hydrogen in the solid state.