First-principles density functional theory (DFT) simulations of various novel 2D materials for energy storage

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Summary:

The discovery of graphene in 2004 and other 2D materials afterwards has generated a new era of materials science with several applications including energy and spintronics. New thin film materials, stable mechanically, thermally and electronically, are available and used for the fabrication of ultrathin flexible devices. The understanding of the properties of, 2D materials, is based on the electronic properties. Modeling and simulation are essential for interpreting the results of the experiments. They are also very useful for predicting the properties of a material even before manufacturing it. Density functional theory (DFT) is one of the most effective and widely used simulation methods in the field of materials. It is a Powerful Quantum mechanics method for the design of 2D Materials. The crystal structure of the material is the only input into these DFT calculations, but even this structure can also be calculated by the DFT. Currently, Density functional theory, helped to make huge advances in the design of emerging materials and nanomaterials for energy conversion and storage.

Indeed, some two dimensional materials are used for energy conversion using photovoltaic effect or as a metal-free water splitting photocatalyst. They are also used for energy storage; as in (Li/Na/Mg)-ion batteries or as solid state materials for hydrogen storage. The solid-state hydrogen storage is based on the interaction between the hydrogen and the surface of the storage material. The storage capabilities of nanostructured materials are high due to their enormous surface area. Moreover, van der Waals (vdW) heterostructures have recently emerged as an additional avenue to engineer new properties by stacking 2D materials in a desired fashion. In this tutorial I will focus on the most promising 2D materials and heterostructures for energy storage.