Hydrogen storage in Metal atoms decorated Boron and Boron-Nitrogen Co-doped graphene

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In the last two decades, the significant efforts have been made to develop alternative energy sources instead of fossil fuels because of increasing CO_2 emissions and the environmental impacts. Besides; hydrogen has been concerned to be an ideal clean energy carrier among the other renewable energy sources because of its environmental friendliness. However, some challenges have to be addressed before hydrogen will become a conventional and commonly available energy carrier. Carbon-based materials such as graphene and carbon nanotubes have been designed for hydrogen storage due to their large surface area, lightweight, and tunable properties. Recently, we proposed a new strategy in which we considered three pure transition metal (TM) atoms or/and a combination of two TM atoms and one alkali earth metal atom (AEM) with high, medium and low hydrogen adsorption energies. These different metal atoms are used to decorate the Boron doped graphene sheet (BDG) and investigated their performance towards hydrogen storage capacity through spillover mechanism using first-principles calculations. Our results indicate that that the activation energies for H atom diffusion are much smaller, indicating that a fast H diffusion on this proposed surface can be achieved. These TM and AEM atoms decorated BDG surface can have the maximum hydrogen gravimetric capacity of 6.4% for double-sided adsorptions. To achieve higher gravimetric density, we also considered the Boron and Nitrogen co-doped graphene surface (BNDG) because B–N pair is isoelectronic to the C–C pair. However, controlling the binding strength of considered metal atoms with that of the BNDG surface is an important issue in the application of hydrogen storage. The recent studies have shown that the binding strength between the metal atom and the substrate can be controlled by means of applying an external electric field. Thus, the effects of the external electric field, as well as the effects of applying point charges on the designed medium towards its hydrogen storage capacity have investigated using density functinoal theory calcualtions.

References:

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