Seminar

Institute for Plasma Research

Title : Experimental and first principal studies on hydrogen desorption behaviour of graphene nanofiber catalyzed MgH_2

Speaker: Dr. Milind Kumar Singh
Banaras Hindu University, Varanasi

Date : 30th July 2021 (Friday)

Time : 03.30 PM

Venue : Online - Join the talk:
https://meet.ipr.res.in/Dr.MilindKumarSingh_PDFTalk

Abstract :

With the combination of experiment and first-principles theory, we have evaluated and explored the catalytic effects of graphitic nanofibers for hydrogen desorption behaviour in magnesium hydride. The helical form of graphene nanofibers, HGNF, with larger surface area, curved configuration and high density of graphene layers resulting in large quantity of exposed carbon sheet edges, are found to considerably improve hydrogen desorbtion from MgH_2 at lower temperatures compared to graphene. Using density functional theory, we find that graphene sheet edges, both the zigzag and armchair type, can weaken Mg−H bonds in magnesium hydride. When the MgH_2 is catalyzed with higher electronegative and reactive graphene edge of graphene, the electron transfer occurs from Mg to carbon, due to which MgH_2 is dissociated into hydrogen and Mg-H component and getting bonded with the graphene edge carbon atoms in the form of C-Mg-H and C-H bonds. In the as formed C-Mg-H, the graphene edges “grab” more electronic charge compared to the normal charge donation of Mg to H, which leads to the weakening of the Mg-H bond, causing hydrogen to desorb at lower temperatures.