"Hydrogen storage in SiC, GeC, and SnC nanocones functionalized with Nickel , DFT – Study"

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Abstract

Hydrogen is regarded as one of the most potential sustainable energy sources in the future. applications including transportation. Still, the event of materials for its storage is difficult notably as a fuel in vehicular transport. Nanocones are a promising hydrogen storage material. Silicon, germanium, and tin carbide nanocones have recently been proposed as promising hydrogen storage materials. In the present study, we have investigated the hydrogen storage capacity of iC,GeC and SnC nanocones functionalized with Ni. The functionalized Ni a are found to be adsorbed on iCNC,GeCNC and SnCNC with an adsorption energy of -5.56, -6.70 and -4.25 eV. The functionalized iCNC,GeCNC and SnCNC bind up to seven, six and four molecules of hydrogen with the adsorption energy of (-0.34, -0.35 and -0.26 eV) and an average desorption temperature of around 434, 447 and 332K (ideal for fuel cell applications). The SiC, GeC, and SnC nanocones systems exhibit a maximum gravimetric storage capacity of 12.51, 7.78 and 4.08 wt%. We suggested that Ni- SiCNC and Ni- GeCNC systems can act as potential H2 storage device materials because of their higher H2 uptake capacity as well as there with strong interaction adsorbed hydrogen molecules than Ni-SnCNC systems. The hydrogen storage reactions are characterized in terms of the charge transfer, the partial density of states (PDOS), frontier orbital band gaps, isosurface plots, and electrophilicity are calculated for the functionalized and hydrogenated SiC,GeC and SnC nanocones.

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