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First Principles Study of Vanadium decorated Graphene; effect on hydrogen storage and H2S sensing.

We conducted theoretical investigation of the structural and electronic properties of Vanadium- functionalized graphene and its effect on hydrogen storage and H2S sensing. Vanadium (V) was an effective addition required for enhancing the properties of graphene sheet. In fact, we found that up to four H2 molecules could be adsorbed by V-functionalized graphene with an average binding energy between 0.966–0.683 eV. Our calculations predicted that the adsorption energy of H2S molecule near the V/graphene (2.192 eV) is remarkably higher (by ˜5.0 times) than that on the pristine graphene (0.490 eV), indicating that Vanadium decoration could significantly enlarge the interactions between adsorbate and adsorbent. Then, our results also predict V-functionalized graphene is a potential hydrogen storage medium and H2S sensing for on-board applications.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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