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Catalytically and chemically modified reduced graphene oxide composites for room temperature hydrogen storage

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The key mechanism for successful hydrogen storage would include an optimum bonding strength between the incoming H_2 gas molecules and the adsorbent. It should be sufficiently strong to result in a stable thermodynamic state while also being moderately weak to release hydrogen with a small increase in temperature [1]. To this end, composites consisting of nanostructured Pd_3Co and MgNi alloy supported on nitrogen/boron (N/B) doped reduced graphene oxide (rGO) have been synthesized. These composites exhibit appreciable hydrogen storage capacity at room temperature and equilibrium hydrogen gas pressure of 3 MPa [2,3]. The synergistic effects of nanostructuring and alloying, their dispersion on graphene (G) and boron/nitrogen doped graphene have been explored. This helps to understand the varying hydrogen bonding strengths and their effect on subsequent adsorption capacities. It is observed that at moderate pressures of 3 MPa and room temperature, Pd_3Co alloy nanoparticles supported on nitrogen doped rGO (NG) and $MgNi_2$ alloy nanoparticles supported on NG exhibit a hydrogen storage capacity of 4.2 wt. % and 5.4 wt. %, respectively. The underlying mechanism for achieving high hydrogen storage is understood using first principle DFT calculations and corroborated by experimental results. Thus, the insights obtained from these studies can be effectively used for developing potential hydrogen storage materials that meet the DOE targets.

References:

[1] Rupali Nagar, B.P.Vinayan, Sai Smruti Samantaray and Sundara Ramaprabhu, "Recent advances in hydrogen storage using catalytically and chemically modified graphene nanocomposites ", Journal of Material Chemistry A 5 (2017) 22897-22912.
[2] Sai Smruti Samantaray, Sangeeta.V, Abhinaya. S and Sundara Ramaprabhu, "Enhanced hydrogen storage performance in Pd3Co decorated nitrogen/boron doped graphene composites ", International Journal of Hydrogen Energy 43 (2018) 8018–8025.
[3] Sai Smruti Samantaray, Sangeeta.V, Abhinaya. S and Sundara Ramaprabhu, "Diatom frustule-graphene based nanomaterial for room temperature hydrogen storage", International Journal of Hydrogen Energy 45 (2019) 764–773.

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