Title

Adsorption of a Ni single atom catalyst on a pristine nanographene (coronene) and H-H activation. A theoretical study of Ni-SAC

Abstract

A computational study of a Ni atom in a coronene (Cor) molecule, as a model of a single-atom catalyst (SAC), was carried out using a DFT approach. The adsorption energy results of Ni on Cor (2.31–1.84 eV) are similar to those reported for extended graphene. Ni-Cor adsorption is preferred at edge sites and electron transfer from Ni to Cor occurs. H2 adsorbs on Ni-Cor with 1.03–1.24 eV. Correlations were obtained between the H2 adsorption energies and some properties of Ni-Cor. The results suggest that Ni-Cor could be used for hydrogen storage and also for catalytic hydrogenation of hydrocarbons. © 2024

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