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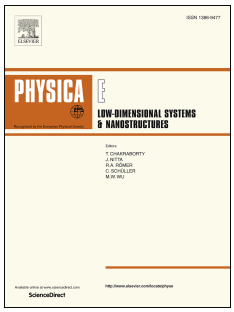

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Hydrogen bonding-mediated dehydrogenation in the ammonia borane combined graphene oxide systems

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Abstract

The dehydrogenation of ammonia borane (AB) adsorbed on three different graphene oxide (GO) sheets is investigated within the *ab initio* density functional theory. The energy barriers to direct combination the hydrogens of hydroxyl groups and the hydridic hydrogens of AB to release H_2 are relatively high, indicating that the process is energetically unfavorable. Our theoretical study demonstrates that the dehydrogenation mechanism of the AB-GO systems has undergone two critical steps, first, there is the formation of the hydrogen bond (O–H–O) between two hydroxyl groups, and then, the hydrogen bond further react with the hydridic hydrogens of AB to release H_2 with low reaction barriers.

Keywords:
Dehydrogenation; AB-GO systems; Hydrogen bond

1. Introduction

Hydrogen is believed to be an ideal energy carrier because of its clean, abundance, and environmental friendliness[1, 2]. The search for novel hydrogen storage materials that can store hydrogen with high gravimetric and volumetric density under ambient thermodynamic conditions is a critical issue for many scientific workers. Recently, ammonia borane(NH_3BH_3, AB)

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