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A computational study of hydrogen adsorption on penta-NiN_2 sheet and nanotubes

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HIGHLIGHTS

- Penta-sheet and nanotube for hydrogen storage.
- Each Ni site in the penta-NiN_2 sheet can only adsorb two H_2 molecules.
- The perfect penta-NiN_2 sheet can't reach the DOE target for H_2 storage.
- N-vacancy, Ni replacement, and grain boundary need to be introduced to enhance the adsorption energy and capacity.

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ABSTRACT

Stimulated by the recent synthesis of penta-NiN_2 sheet [ACS Nano 2021, 15, 13,539], we study the hydrogen adsorption on the sheet and the derived nanotubes by using density functional theory with the correction of van der Waals interactions. We have found that each Ni site can only adsorb two hydrogen molecules as expected from the 18-electron rule, the corresponding capacity is 4.44 wt%. As more H_2 molecules are introduced, H_2 can only be very weakly adsorbed on N sites. When the sheet is curved into nanotubes, the Ni–N distance is enlarged due to the stress, which weakens the orbital hybridizations between Ni and N, and reduces the charge transfer from Ni to N. The Ni ion with a less charge on the tube shows weak polarizing ability for H_2 molecule.

Introduction

Solid materials for hydrogen storage via absorption and adsorption are of current interest as required by the green renewable energy technology. Materials suitable for hydrogen storage must meet specific requirements, such as an optimal adsorption energy window (0.1–0.6 eV/H_2) [1], and high gravimetric (5.5%) and volumetric (40 g/L) capacity targets set by the United States Department of Energy [2]. However, it is challenging to reach these targets, which motivates scientists to design new materials.

Since the proposal of penta-graphene (PG) [3], pentagon becomes an important structural unit that has led to a paradigm shift in new materials design and synthesis. So far, more than 150 penta-sheets have been proposed [4] exhibiting unique geometry and novel properties as compared with graphene, MXene, black phosphorus, dichalcogenides, and trichalcogenides. Pentagon-based 2D sheets significantly expanded the 2D materials family with additional new

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