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Review

Review on Tuning the Dimensionality and Geometry of Metal Nitride and Boride Nanostructures for Enhanced Hydrogen Storage: Advances and Outlook

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ABSTRACT: Hydrogen is an abundant and clean energy carrier, yet efficient and safe storage remains a major obstacle to the realization of a sustainable hydrogen economy. Conventional storage technologies based on high-pressure compression and cryogenic liquefaction still struggle to satisfy the operational safety and economic viability. Solid-state hydrogen storage offers a promising alternative; however, achieving reversible hydrogen adsorption under near-ambient conditions with sufficiently high storage capacity remains a significant challenge. In this minireview, we demonstrate that nanostructuring, particularly through controlling the dimensionality and geometry of metal-nitride- and boride-based nanostructures, provides an effective strategy for tuning hydrogen adsorption energies into the optimal range from approximately −0.2 to −0.6 eV/H_2 required for reversible storage. We systematically discuss how dimensionality, curvature, pore geometry, and local coordination environments influence hydrogen adsorption mechanisms, active-site stability, and storage performance by regulating charge transfer, orbital hybridization, local electric fields, and hydrogen-binding strength. We also analyze the critical roles of strain engineering, defect engineering, and metal-site stabilization in optimizing adsorption/desorption thermodynamics and suppressing metal clustering. These insights establish a comprehensive structure−property relationship framework for balancing storage capacity, adsorption energetics, reversibility, and kinetics.

1. INTRODUCTION

The world population is expected to reach 9.7 billion in 2050, leading to a significant increase in energy demand.[1] Currently, fossil fuels such as oil, coal, and natural gas supply over 80% of the world's energy.[2,3] As populations grow and energy use rises, transitioning to clean and renewable energy sources, like solar, wind, and hydropower, is urgently needed. This shift is crucial to reducing the environmental harm caused by fossil fuels and achieving a sustainable energy future.[4]

Hydrogen has the highest gravimetric energy density of any fuel 120 MJ/kg, three times that of gasoline. However, at standard temperature (25 °C) and pressure (1 bar), hydrogen has a very low density (0.0824 kg/m^3) and low volumetric energy density (0.01 MJ/L of H_2), making storage and transportation challenging.[5] Despite this drawback, hydrogen offers a significant environmental advantage as it produces only water vapor and emits no greenhouse gases when used as an energy carrier. This makes hydrogen a promising candidate for addressing global energy demands and mitigating environmental challenges.

The hydrogen cycle begins with sunlight being converted into electricity via solar panels. This electricity is then used to split water into hydrogen and oxygen through electrolysis. The oxygen is released into the atmosphere, while the hydrogen is stored, transported, and utilized for various applications. When hydrogen reacts with oxygen during combustion or in fuel cells, it releases energy in the form of heat and work, producing only water or steam as a byproduct. This creates a closed and sustainable cycle, as illustrated in Figure 1.[6]

Hydrogen storage is a critical challenge in the development of a hydrogen economy. The U.S. Department of Energy (DOE) has established specific targets for storage capacity, as outlined in Table 1.[7] Traditional storage methods, such as compressing hydrogen gas at high pressures or liquefying it at very low temperatures, are costly and raise safety concerns.[8] However, these methods face limitations, including low capacity, complex processes for hydrogen addition and

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