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First-Principles Insights into Defect-Engineered BN Semiconductors for Efficient Green Hydrogen Generation and Sustainable Energy Storage

Bo_Sheng Chen[1], Hung-Lung Chou[1,2,*], Ting-Wen Lai[1]
[1] Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology,
P. O. Box 106, Taipei, Taiwan
[2] Institute of Applied Sustainable Energy Technology, National Taiwan University of Science and Technology,
P. O. Box 106, Taipei, Taiwan
*Presenter:Bo-Sheng Chen, Presenter's e-mail: m11222604@mail.ntust.edu.tw
*Corresponding author's e-mail: HLCHOU@mail.ntust.edu.tw

Abstract

The pursuit of renewable energy solutions is a critical priority in the context of global energy transition. Among these, hydrogen has emerged as a promising green energy carrier due to its high efficiency, environmental compatibility, and multifunctionality. When utilized in combustion or fuel cell applications, hydrogen (H_2) produces only water as a byproduct, making it a truly zero-carbon energy source without greenhouse gas emissions or pollutants[1-5]. However, the sustainability of hydrogen depends largely on its production pathway. Currently, hydrogen is primarily produced via three methods: gray hydrogen (from fossil fuels with high CO_2 emissions), blue hydrogen (with carbon capture and storage to mitigate emissions), and green hydrogen—the most sustainable route—generated through water electrolysis powered by renewable energy.In addition to its clean profile, hydrogen offers potential as a long-term energy storage medium, addressing the intermittency of renewable sources such as solar and wind. Nonetheless, widespread adoption of green hydrogen still faces challenges including high production costs, limited infrastructure, and relatively low energy conversion efficiency. Overcoming these hurdles requires continuous technological innovation and cost-effective strategies[6-9].

In this study, density functional theory (DFT) simulations are employed to investigate hydrogen generation via water splitting on defect-engineered hexagonal boron nitride (h-BN) surfaces. By analyzing charge density distributions and partial density of states (PDOS), this research identifies the most catalytically active defect configurations. The findings offer theoretical insights into the design of efficient hydrogen evolution catalysts and provide a promising strategy for future green hydrogen production and energy storage technologies.

First-principles calculations revealed that boron-deficient hexagonal boron nitride (h-BN) nanosheets exhibit superior catalytic performance in hydrogen production via water splitting. The presence of boron vacancies introduces additional active sites, significantly lowering the energy barrier for water dissociation (e.g., T.S. energy of 1.52 eV), thereby facilitating O–H bond cleavage and subsequent hydrogen release. In contrast, nitrogen-deficient systems offer fewer reactive sites, and water molecules tend to form stable two-dimensional planar structures, leading to higher reaction barriers (e.g., T.S. energy of 2.61 eV). These findings underscore the critical role of defect engineering in tuning catalytic properties and highlight the potential of h-BN as a next-generation hydrogen storage material. This work provides a promising theoretical basis for the design of efficient catalysts aimed at green hydrogen production and contributes to the broader goal of sustainable energy development.

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