

Improving MgH_2 hydrogen storage with oxygen vacancy-enriched $H\text{-}V_2O_5$ nanosheets as an active H-pump

May 22 2024



Credit: Nano-Micro Letters (2024). DOI: 10.1007/s40820-024-01375-8



With the depletion of fossil fuels and global warming, there is an urgent need to seek green, clean, and efficient energy resources. Against this backdrop, hydrogen is considered a potential candidate for replacing fossil fuels due to its high energy density and environmentally friendly nature. To realize the development of a hydrogen economy, safe and efficient hydrogen storage technologies are crucial.

Compared to traditional compressed hydrogen and cryogenic liquid hydrogen storage technologies, solid-state hydrogen storage is considered a safer and more efficient method. Magnesium hydride (MgH₂), as one of the most promising solid-state hydrogen storage materials, has attracted attention due to its abundant elemental resources, high hydrogen storage capacity, good reversibility, and non-toxicity. However, the relatively high operating temperature of MgH₂ limits its large-scale commercial application in vehicular or stationary hydrogen storage.

Introducing transition metal-based catalysts with unique three-dimensional electronic structures is considered an effective method to improve the kinetics of MgH₂. Vanadium (V) and its oxides are often used as catalysts for MgH₂ due to their multivalence and high catalytic activity. However, due to the high ductility of metallic vanadium and relatively low activity, vanadium-based oxides have broader application prospects.

Layered V_2O_5 with a layered structure is one of the promising catalysts to enhance the hydrogen storage performance of MgH₂/Mg, but limited catalytic capacity due to insufficient contact between V_2O_5 and MgH₂.

To address this issue, Dr. Jianxin Zou's team at Shanghai Jiao Tong University employed a solvothermal method followed by subsequent hydrogenation to prepare ultra-thin hydrogenated V_2O_5 nanosheets with abundant oxygen vacancies and used them as catalysts to improve the



hydrogen storage performance of MgH₂.

The study is <u>published</u> in the journal *Nano-Micro Letters*.

The MgH₂-H-V₂O₅ composite material exhibits excellent hydrogen storage performance, including a lower desorption temperature ($T_{onset} = 185^{\circ}C$), rapid desorption kinetics ($E_a = 84.55 \text{ kJ mol}^{-1} \text{ H}_2 \text{ for}$ desorption), and long-term cyclic stability (capacity retention of up to 99% after 100 cycles). Particularly, the MgH₂-H-V₂O₅ composite material shows outstanding hydrogen absorption performance at room temperature, with a hydrogen absorption capacity of 2.38 wt% within 60 minutes at 30°C.

The $H-V_2O_5$ nanosheets synthesized by Dr. Zou's team possess a unique two-dimensional structure and abundant oxygen vacancies, enabling the in-situ formation of V/VH_2 during the reaction process, all of which contribute to enhancing the hydrogen storage performance of MgH_2 .

By using a solvothermal method to create a distinct anisotropic layered structure, a highly exposed surface is formed, thereby providing more active sites and pathways for hydrogen/electron diffusion, thus improving hydrogen storage performance. Moreover, crucially, the presence of oxygen vacancies accelerates electron transfer, stimulating the "hydrogen pump" effect of VH₂/V, facilitating the dehydrogenation of VH₂ and MgH₂, and reducing the energy barriers for hydrogen dissociation and recombination.

Introducing oxygen vacancy defect engineering into the catalyst thus opens up a new avenue for enhancing the cyclic stability and kinetic performance of MgH₂.



More information: Li Ren et al, Boosting Hydrogen Storage Performance of MgH2 by Oxygen Vacancy-Rich H-V2O5 Nanosheet as an Excited H-Pump, *Nano-Micro Letters* (2024). DOI: 10.1007/s40820-024-01375-8

Provided by Shanghai Jiao Tong University Journal Center

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