

Nanostructured metal hydrides for hydrogen storage

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Metal hydrides are promising candidates for on-board hydrogen storage to meet the ever-growing demands for carbon neutralization. Their high volumetric capacity and safety are advantageous, but the poor kinetics and high operation temperature should be addressed to alternate state-of-the-art cryogenic or 700 bar-compressed hydrogen gas that are necessitating expensive composite tanks. Encapsulation or scaffolding technology shows potential to accelerate the hydrogen storage kinetics by stabilizing metal hydride nanoparticles and catalyzing reactions [1]. Understanding key parameters and the associated governing mechanisms are crucial to optimize the performance of metal hydrides for hydrogen storage.

In this presentation, we will show examples of nanostructured metal hydrides: altering the reaction enthalpy by the chemomechanical interactions between metal hydride and encapsulant [2], bypassing unwanted reaction intermediate by nano-interface engineering [3], and selective synthesis of nanoparticle polymorphs via controlled nucleation kinetics [4]. Our studies emphasize the promise of nanostructured metal hydrides by independently tuning material properties to optimize thermodynamics and kinetics of hydrogen storage, opening new avenues that could lead to the next generation of solid-state materials for hydrogen storage applications.

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[3] Brandon C. Wood, Vitalie Stavila, Natchapol Poonyayant, et al. Nanointerface-driven reversible hydrogen storage in the nanoconfined Li–N–H system. *Adv. Mater. Interfaces*. 2017; 4: 1600803.

[4] Sohee Jeong, Tae Wook Heo, Julia Oktawiec, et al. A mechanistic analysis of phase evolution and hydrogen storage behavior in nanocrystalline Mg(BH₄)₂ within reduced graphene oxide. *ACS Nano*. 2020; 14 (2): 1745.

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