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Composite Boron Nitride-based Immobilized Nanohydride Toward Self-Accelerated Reversible Hydrogen Storage

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Metal hydrides for on-board hydrogen storage play a key role in future conversion of the world to a "hydrogen economy". Nano-structuring these materials proves an effective strategy which can simultaneously enhance their ab/de-sorption thermodynamics and kinetics. However, strategies to combine catalysis and nanoconfinement for controlling factors governing their interfacial hydrogen uptake and release processes are still lacking. In this study, we show how thermal emitting method can be used for generating Mo2N sites to create electron-deficient boron and N-vacancies in inert boron nitride host for LiBH4 activation. The generated Mo2N sites resulted in a shift of the electronic band structure of the host which weakened the Li-B bond of nanostructured LiBH4 species. We demonstrate the tailoring of a strong Mo2N–DBN hybrid structure and clarify the mechanistic origin of its activity. Both experimental results and DFT investigations indicate a long-range interaction of Li in the immobilized nanohydride with B atoms, which optimizes the adsorption energy for absent LiBH4 phase transition and melting upon cycling. This study provides an approach to finely control the host–guest nanointerface interactions of metal borohydride and scaffolds at the atomic level and is expected to guide smart thermodynamic or kinetic alteration of solid-state hydride materials.
Keywords: Density functional theory, Hydrogen economy, adsorption, storage, interfacial charge transfer, nanointerface interactions, electronic band structure, nanoconfinement, thermodynamic or kinetic alteration.

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