In Situ Hybridization of LiNH₂-LiH-Mg(BH₄)₂ Nano-composite: Intermediate and Optimized Hydrogenation Properties

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Fig. S1 TPD results of as-prepared LiNH₂-LiH-0.5Mg(BH₄)₂ samples measured at 5 deg min⁻¹ under argon flow: (red) plasma metal reaction followed by nucleation growth method, (black) traditional ball milling method.



Fig. S2 SEM image of as-prepared LiNH₂-LiH-2Mg(BH₄)₂ nano-composite.



Fig. S3 MS result associate with TPD measured at 5 deg min⁻¹ under argon flow for nano-sized LiNH₂-LiH.



Fig. S4 DSC curves of LiNH₂-LiH-0.5Mg(BH₄)₂ composite at a heating rate of 5, 10 and 20 deg min⁻¹ under Argon.

(Fig. S4)

This LiNH₂-LiH-0.5Mg(BH₄)₂ composite is prepared using high-energy ball milling. The material (Fig. 3b) shows morphology of disordered arrangement, with an average size of 4 μ m. The enthalpies of the three steps are 15.6±1.3, 42.4±3.6, 33.6±2.8 kJ/mol, while the activation energies are 82.5±2.8, 24.6±3.6, 48.9±5.1 kJ/mol. The thermodynamic and kinetic parameters of the bulk sample show that the nanoparticles are beneficial to optimize dehydrogenation performances.