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The enhanced hydrogen storage combination of $6Mg(NH_2)_2$-$9LiH$-$LiBH_4$ observed in (Mg-B-N-H)-doped $Mg(NH_2)_2$-$2LiH$ system

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Doping $Mg(NH_2)_2$-$2LiH$ by 0.1mol $Mg_2(BH_4)_2(NH_2)_2$ compound exhibits enhanced hydrogen de/re-hydrogenation performance. The peak width in temperature-programmed desorption (TPD) profile for the $Mg(NH_2)_2$-$2LiH$-$0.1Mg_2(BH_4)_2(NH_2)_2$ was remarkably shrunk by 60°C from that of pristine $Mg(NH_2)_2$-$2LiH$, and the peak temperature was lowered by 12°C from the latter. Its isothermal dehydrogenation rate was greatly improved by five times from the latter at 200°C. XRD, FTIR and NMR analyses revealed that a series of reactions occurred in the dehydrogenation of the composite. The prior interaction between LiH and Mg-B-N-H yielded intermediate $LiBH_4$, Mg_3N_2 and $Li_2Mg(NH)_2$, which can be described by a merged reaction of $6LiH + 2\ Mg(BH_4)_2$-$Mg(NH_2)_2 \rightarrow 4LiBH_4 + Mg_3N_2 + Li_2Mg(NH)_2 + 6H_2\uparrow$. The $LiBH_4$ and Mg_3N_2 phases can be regarded as the meditation product between LiH with $Mg(BH_4)_2$, and the rapidly subsequent reaction product between intermediate MgH_2 with $Mg(NH_2)_2$, respectively. $Li_2Mg(NH)_2$ was generated from the interaction between LiH and $Mg(NH_2)_2$. Only a few $Mg(NH_2)_2$ joined in the reaction with LiH/MgH_2 but most was remained until the temperature was lifted to 180°C.

The formed $LiBH_4$ subsequently reacted with $Mg(NH_2)_2$ and LiH in molar ratio of 1:6:9 to form $Li_2Mg_2(NH)_3$ and $Li_4BN_3H_{10}$ phases. The observed $6Mg(NH_2)_2$-$9LiH$-$LiBH_4$ combination dominated the hydrogen release and soak in the $Mg(NH_2)_2$-$2LiH$-$0.1Mg_2(BH_4)_2(NH_2)_2$ system. Such combination can be reflected by $6Mg(NH_2)_2 + 9LiH + LiBH_4 \rightarrow Li_4(BH_4)(NH_2)_3 + 3\ Li_2Mg_2(NH)_3 + 9H_2\uparrow$, which is thermodynamically reversible. It can be found that the thermal stability of the reversible system $2Mg(NH_2)_2$-$3LiH$ / $Li_2Mg_2(NH)_3$-$LiNH_2$ was effectively altered by doping 1/3 mol $LiBH_4$. The kinetics of the system was also enhanced by additive $LiBH_4$.

Keywords**:** Hydrogen storage; Mg-B-N-H compounds; Kinetics; Doped $Mg(NH_2)_2$-$2LiH$ system