Improved kinetics of $Mg(NH_2)_2$−2LiH system by addition of lithium halides

Hujun Cao[ab], Han Wang[b], Teng He[b*], Guotao Wu[b], Zhitao Xiong[b], Jieshan Qiu[a], Ping Chen[bc*]

[a] *Carbon Research Laboratory, Liaoning Key Lab for Energy Materials and Chemical Engineering, State Key Lab of Fine Chemicals, Dalian University of Technology, Dalian 116024, P. R. China.*

b Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, P. R. China.

[c] *State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, P. R. China.*

** E−mail: heteng@dicp.ac.cn, Tel: +86−411−84379583, Fax: +86−411−84379583*

** E−mail: pchen@dicp.ac.cn, Tel: +86−411−84379905, Fax: +86−411−84379583*

Supporting information

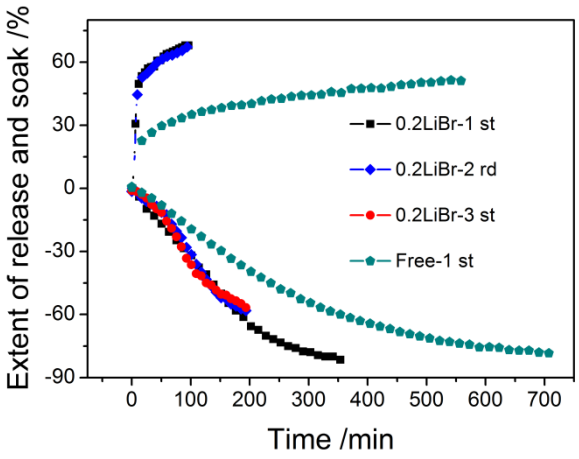

Fig S1. 3 times of isothermal hydrogen desorption and 2 times of isothermal hydrogen absorption of 0.2 LiBr-doped sample at 140 ºC. (The dehydrogenation/re-hydrogenation rates of 0.2LiBr-doped sample at 140 ºC can be hardly reduced).

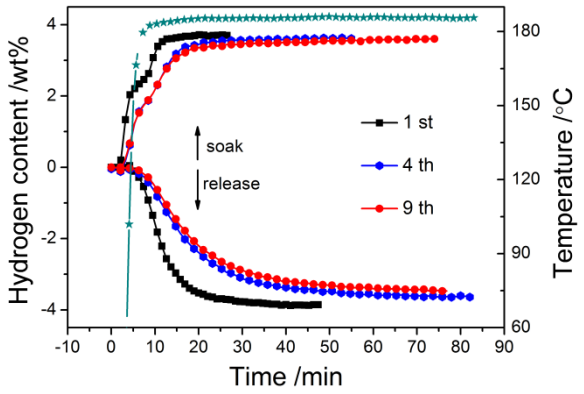

Fig S2. The first, fourth and ninth isothermal hydrogen desorption/absorption cycles of 0.2LiBr-doped sample. (The ninth cycle remains the same hydrogen storage properties as the fourth one).

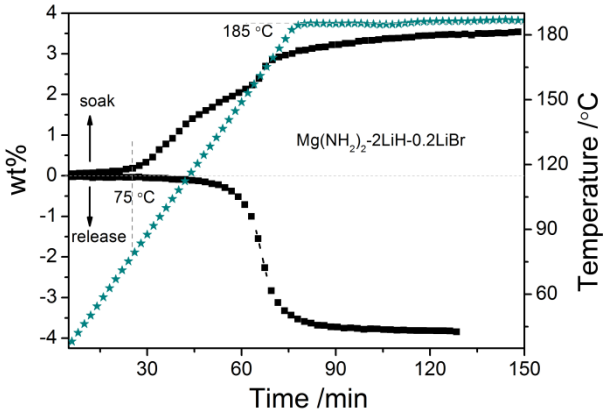

Fig S3. Temperature programmed volumetric release and subsequent soak measurements on the 0.2LiBr-doped sample of the first cycle. (The onset temperature of 0.2LiBr-doped sample is 75 ºC, which is about 20 ºC lower than that of the $Li_2Mg(NH)_2$ sample. Reference: *Advanced Materials* 2004, ***16***, 1522).

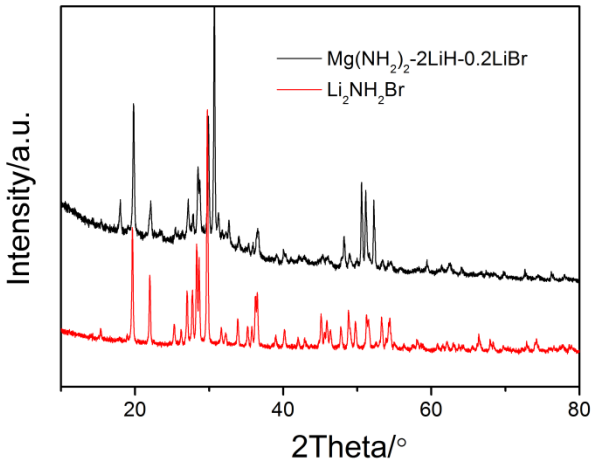

Fig S4. XRD pattern of 0.2LiBr-doped sample after quenching at 200 ºC for 18 h and the as-prepared Li_2NH_2Br samples. (Li_2NH_2Br was prepared according to *Faraday Discuss,* 2011, **151**, 271).

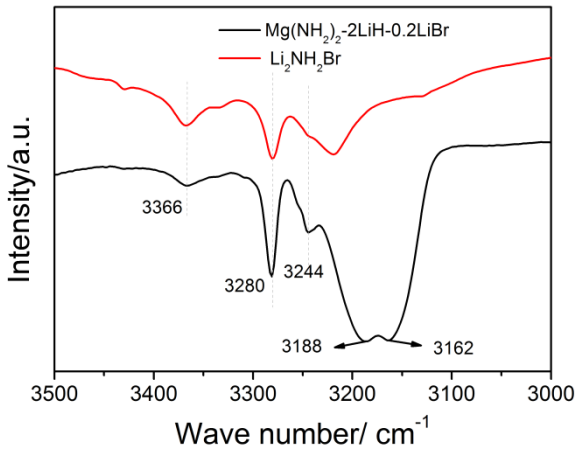

Fig S5. FTIR spectra of 0.2LiBr-doped sample after quenching at 200 ºC for 18 h and the as-prepared Li_2NH_2Br sample.

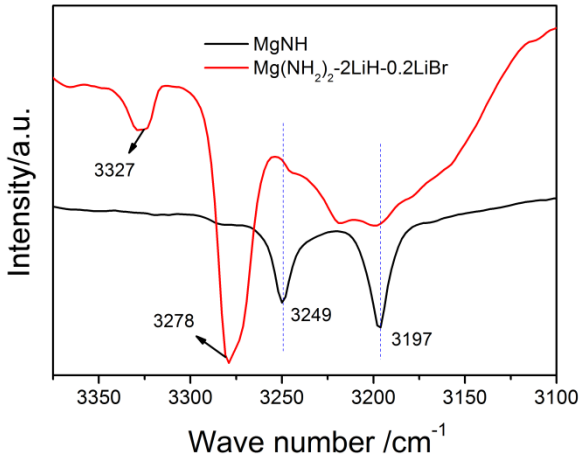

Fig S6. FTIR spectra of 0.2LiBr-doped sample after hydrogenation at 185 ºC and the pure MgNH sample.

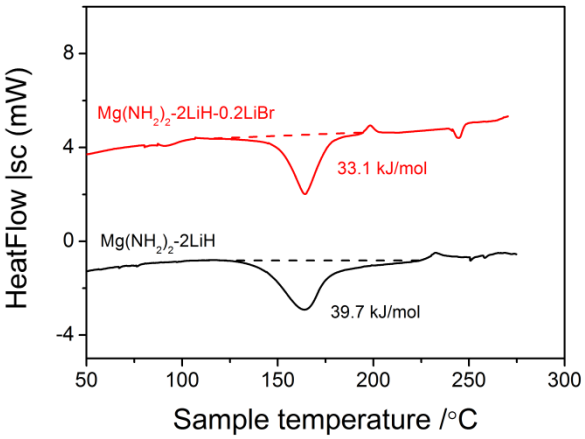

Fig S7. The C80 information of 0.2LiBr-doped and pristine $Mg(NH_2)_2$−2LiH samples. (Differential scanning calorimetry (DSC) measurement was carried out on a SETARAM C80 thermal analysis system equipped with a closed sample cell at a ramping rate of 0.2 K/min. With the C80 result, we can see that the dehydrogenation enthalpy of $Mg(NH_2)_2$−2LiH system was reduced from 39.7 to 33.1 kJ/mol H_2 by addition of 0.2LiBr).