Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information for

Tailoring the hydrogen storage properties of $Li_4BN_3H_{10}$ by confinement into highly ordered nanoporous carbon

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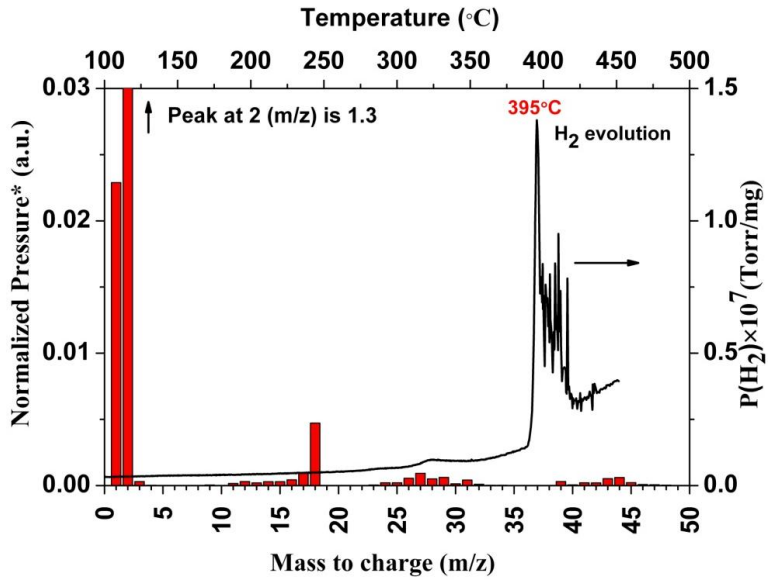
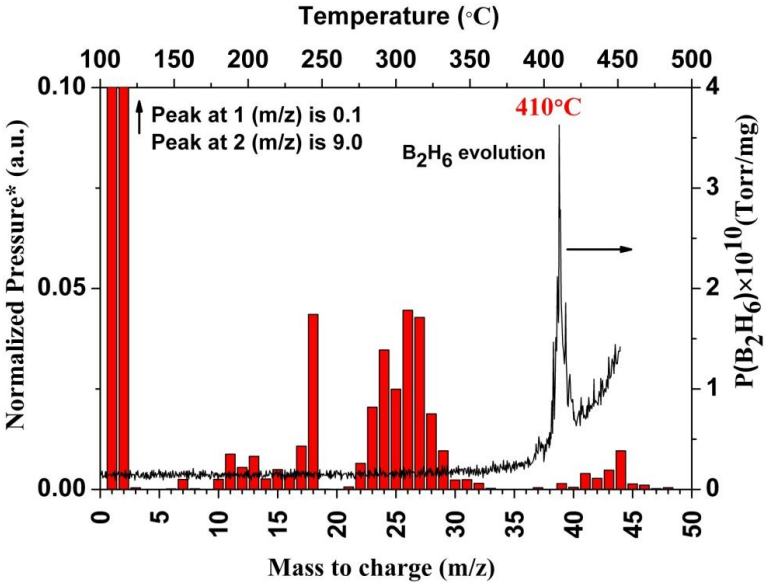


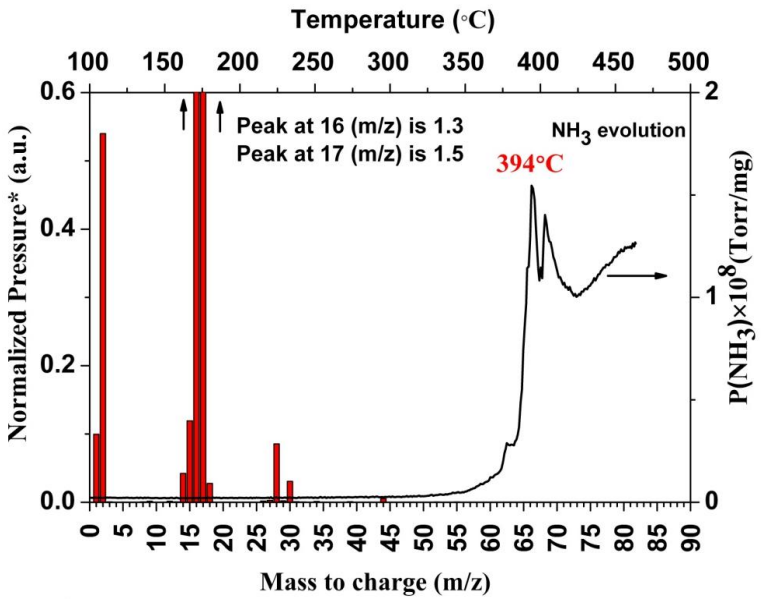
(a)



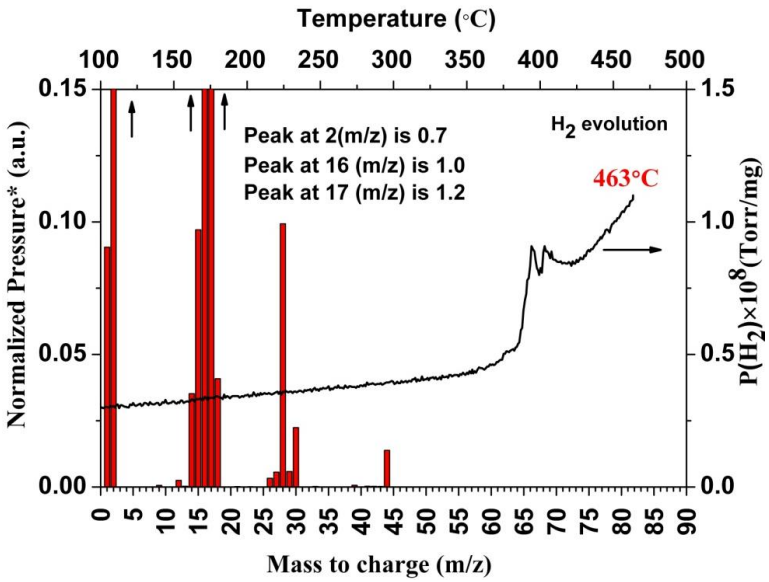
(b)

Fig. S1. Direct line-of-sight RGA cracking patterns and gas evolution of $LiBH_4$. (a) shows the evolution of H_2 (m/z=2) as well as the cracking pattern taken at 395°C; (b) shows the evolution of B_2H_6 (m/z=24) as well as the cracking pattern taken at 410°C.

*All mass spectra bar graphs have been background subtracted. All arbitrary units (a.u.) are with respect to the partial pressure of the corresponding gas evolution.



(a)



(b)

Fig. S2. Direct line-of-sight RGA cracking patterns and gas evolution of $LiNH_2$. (a) shows the evolution of NH_3 (m/z=17) as well as the cracking pattern taken at 394°C; (b) shows the evolution of H_2 (m/z=2) as well as the cracking pattern taken at 463°Cwhich is the near the maximum process temperature. The evolution of hydrogen continues beyond 475°C, but the peaks shown in the hydrogen curve more than likely are hydrogen release associated with the release of ammonia. Present in the ammonia and hydrogen cracking patterns are N_2H_2 (m/z = 28 and 30 at similar ratios).

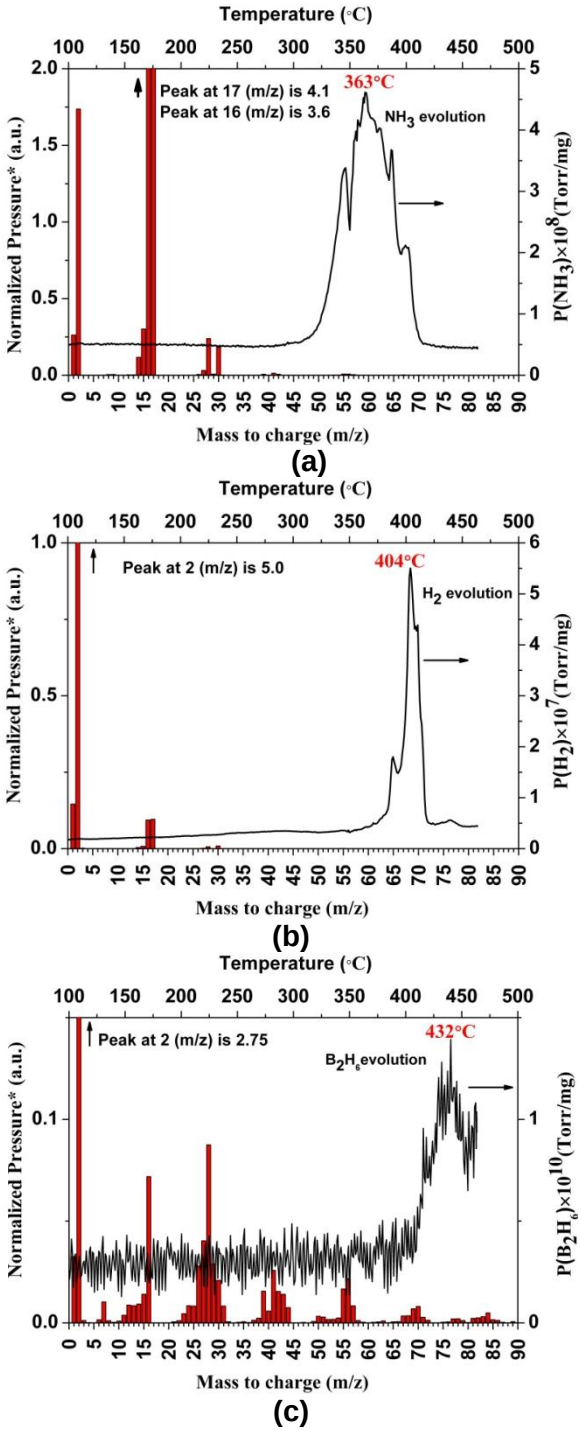


Fig. S3. Direct line-of-sight RGA cracking patterns and gas evolution of $Li_4BN_3H_{10}$. (a) shows the evolution of NH_3 (m/z=17) as well as the cracking pattern taken at 363°C; (b) shows the evolution of H_2 (m/z=2) as well as the cracking pattern taken at 404°C; (c) shows the evolution of B_2H_6 (m/z=24) as well as the cracking pattern taken at 432°C. The evolution of triborane or larger species (possibly even nitrogen containing boranes such as BNH_2 or BNH_3, for example) is evident from the masses between m/z of 39-44 and groups centered at 56 and 69.

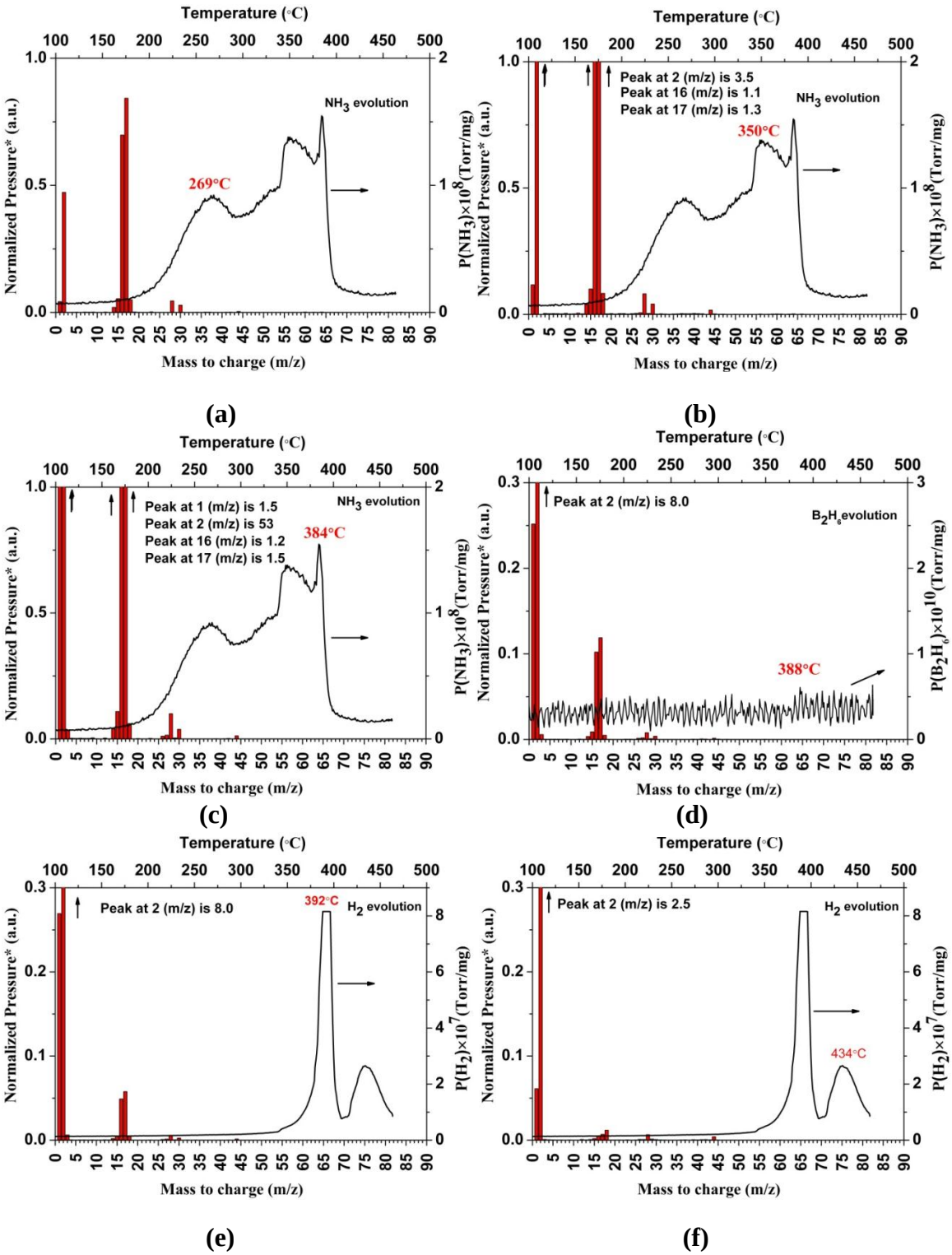


Fig. S4. Direct line-of-sight RGA cracking patterns and gas evolution of $Li_4BN_3H_{10}$@NPC. (a,b,c) shows the evolution of NH_3 (m/z=17) as well as the cracking pattern taken at the three peaks at 269°C, 350°C, 384°C respectively; (d) shows the evolution of B_2H_6 (m/z=24) as well as the cracking pattern taken at 388°C. This cracking pattern is absent any strong signal of triborane

or larger species, especially diborane; (e,f) shows the evolution of H_2 (m/z=2) as well as the cracking pattern taken at the peaks of 392°C and 434°C respectively.