Supporting Information for

Tailoring the hydrogen storage properties of Li$_4$BN$_3$H$_{10}$ by confinement into highly ordered nanoporous carbon

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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$_2$H$_6$ (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.
Fig. S2. Direct line-of-sight RGA cracking patterns and gas evolution of LiNH₂. (a) shows the evolution of NH₃ (m/z=17) as well as the cracking pattern taken at 394°C; (b) shows the evolution of H₂ (m/z=2) as well as the cracking pattern taken at 463°C which 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 N₂H₂ (m/z = 28 and 30 at similar ratios).
Fig. S3. Direct line-of-sight RGA cracking patterns and gas evolution of Li$_4$BN$_3$H$_{10}$. (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$_2$H$_6$ (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 Li₄BN₃H₁₀@NPC. (a,b,c) shows the evolution of NH₃ (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 B₂H₆ (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 H₂ (m/z=2) as well as the cracking pattern taken at the peaks of 392°C and 434°C respectively.