Supporting Information

Effect of Lithium Doping into MIL-53(Al) through Thermal Decomposition of Anion Species on Hydrogen Adsorption

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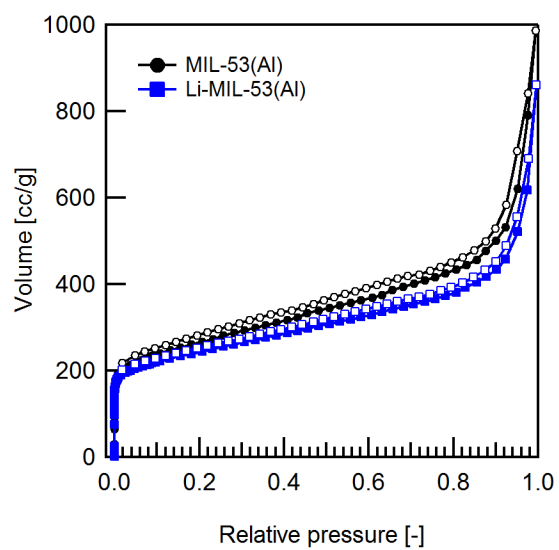
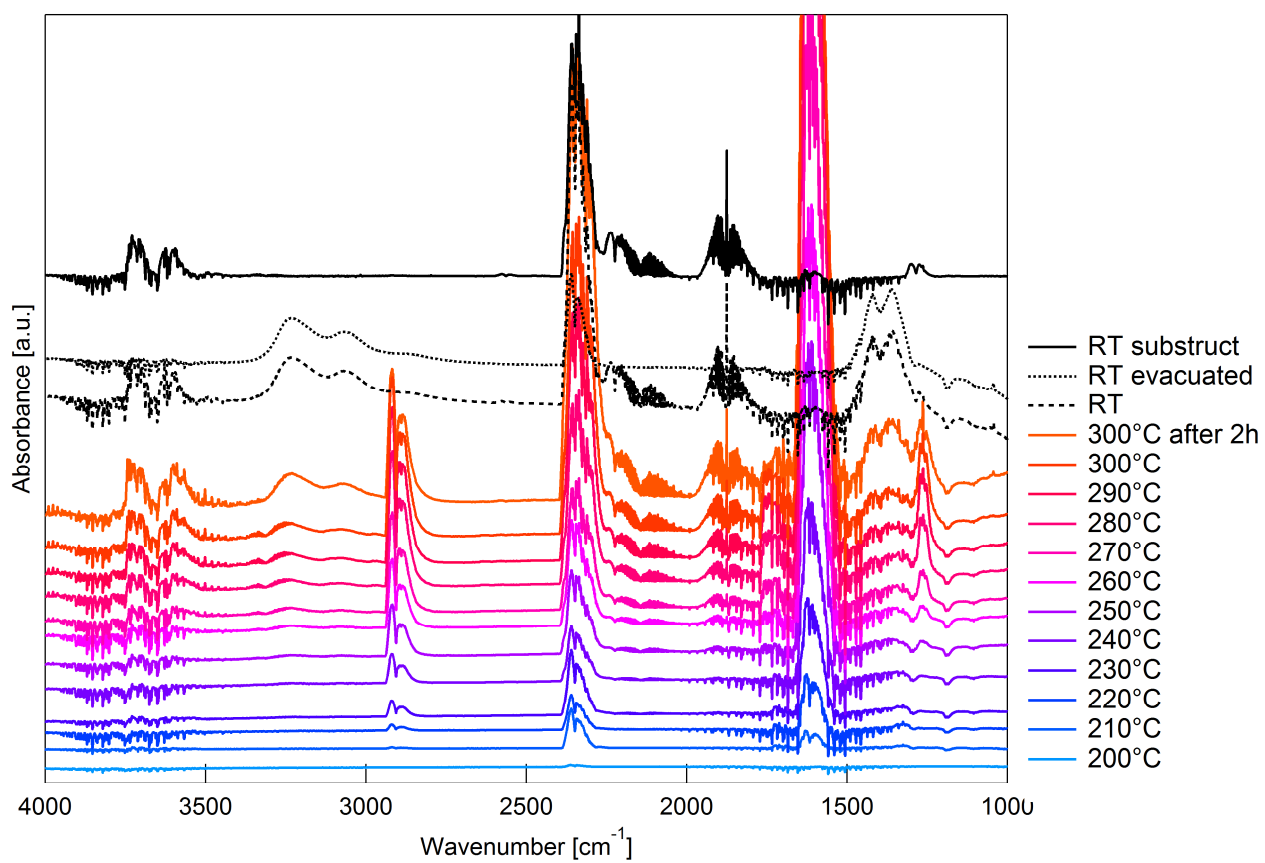**Figure S1.** N2 adsorption isotherms of MIL-53(Al) and Li-MIL-53(Al).

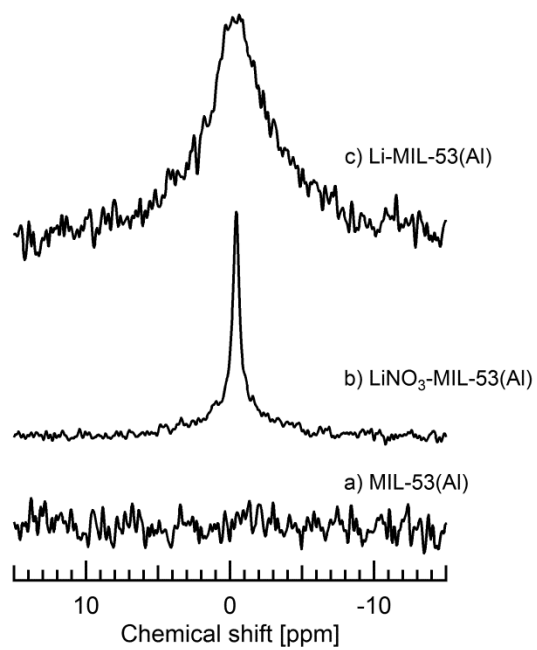**Figure S2.** FT-IR spectra of released gas species from LiNO$_3$-MIL-53(Al) during heating.

c) Li-MIL-53(Al)

b) LiNO$_3$-MIL-53(Al)

a) MIL-53(Al)

10   0   -10
Chemical shift [ppm]

Figure S3. ^{7}Li MAS NMR spectra of a) MIL-53(Al), b) LiNO$_3$-MIL-53(Al), and c) Li-MIL-53(Al).
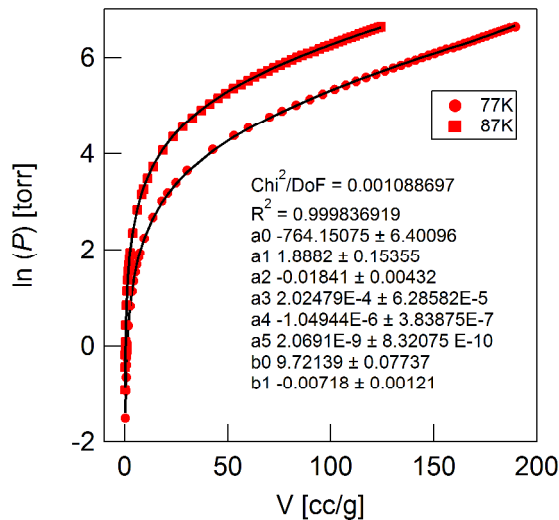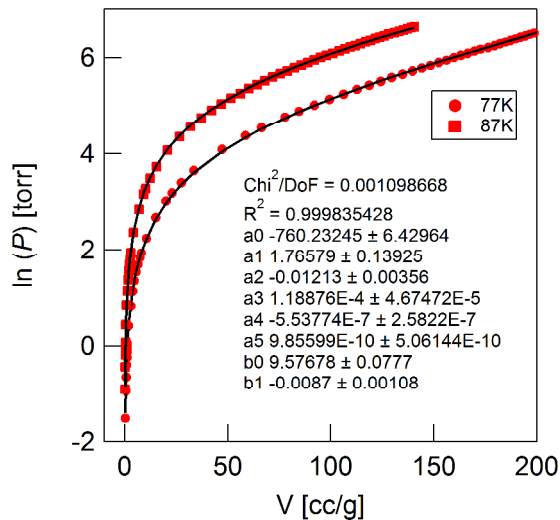
Fig 3.a) MIL-53(Al)

Fig 3.b). Li-MIL-53(Al)

Figure S4. Details of fitting and calculation of isosteric heat of hydrogen adsorption for a) MIL-53(Al) and b) Li-MIL-53(Al).

Both hydrogen isotherms (77K and 87K) for each material were fit to a virial equation of the form given in Equation 1.[S1]

The heat of adsorption is then calculated from the fitting parameters using Equation 2

$$\ln P = \ln N + \frac{1}{T}\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \quad (1)$$

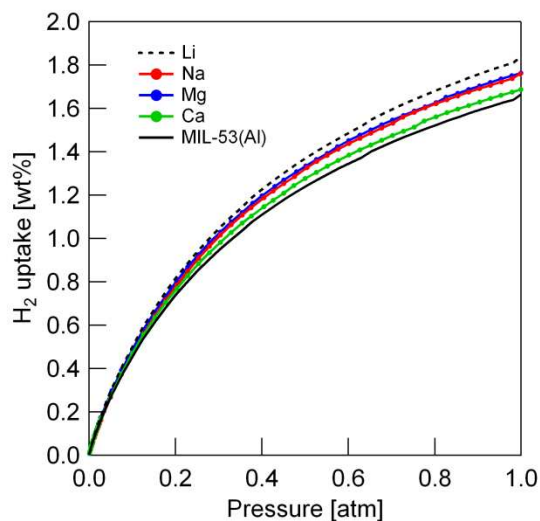$$Q_{st} = -R\sum_{i=0}^{m} a_i N^i \quad (2)$$

Figure S5. Hydrogen adsorption isotherms of other alkaline doped MIL-53(Al) at 77K.

Reference

(S1)   Czepirski, L.; Jagiello, J., *Chem. Eng. Sci.* **1989,** *44*, 797-801.