Supporting Information for:

Improved CO_2 Capture Performances of ZIF-90 through Sequential Reduction and Lithiation Reactions to Form a Hard/Hard Structure

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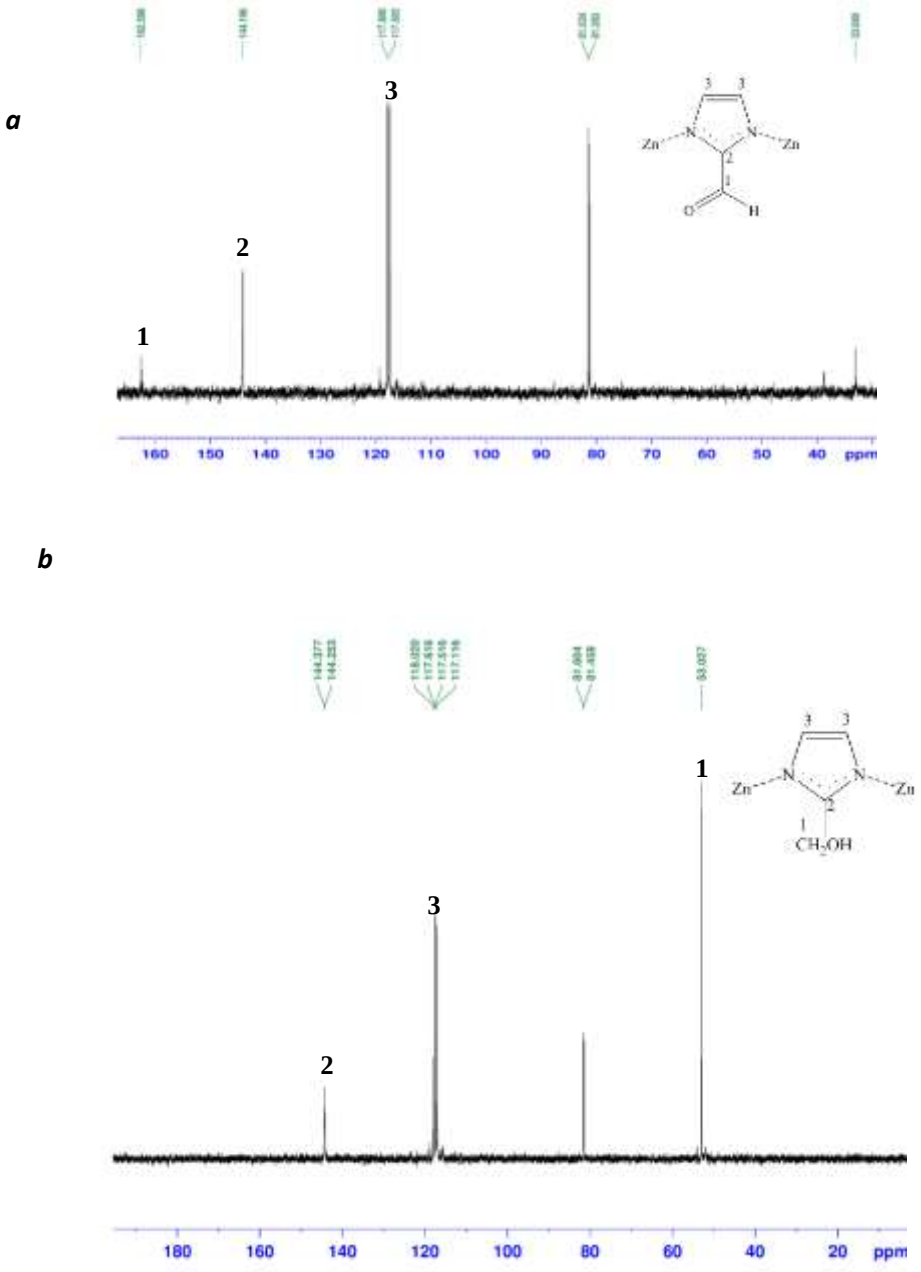

Fig. S1.^{13}C NMR spectrum of the as-synthesizedZIF-90 (a) ZIF-91 (b)

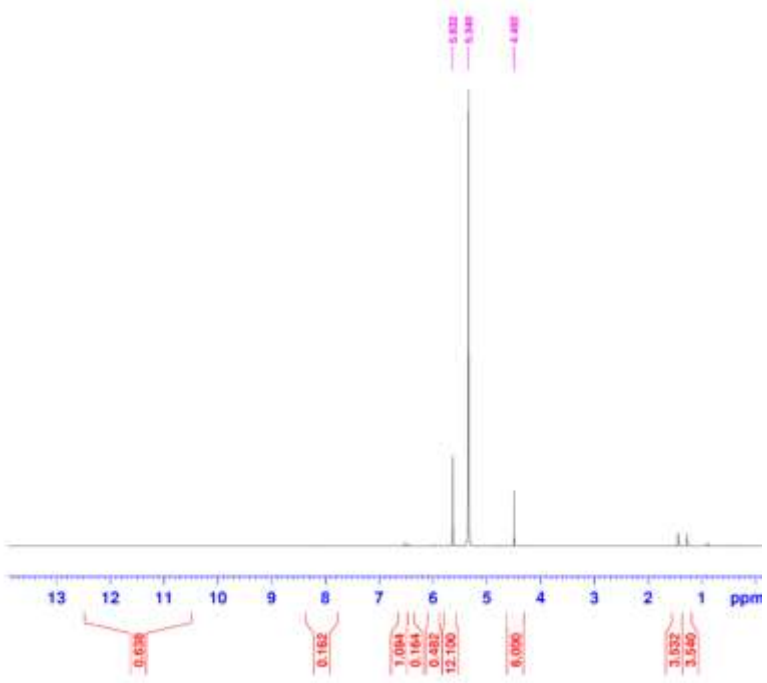

Fig. S2. 1HNMRspectrum of the as-synthesized ZIF-90

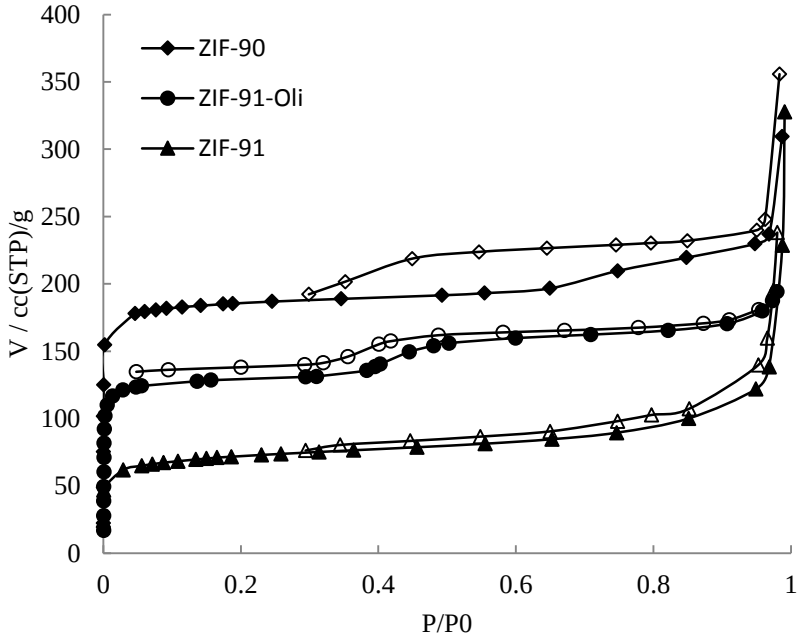

Fig. S3. Nitrogen adsorption-desorption isotherms for ZIF-90, ZIF-91 and ZIF-91-OLi at 77K.

(Filled symbols: Adsorption and Open symbols: Desorption)

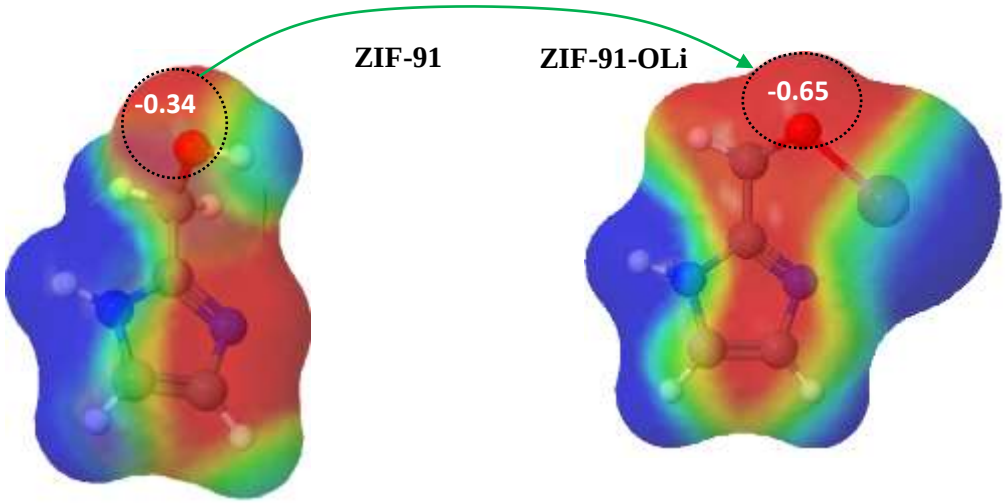

Fig. S4. The calculated MEP surface for ZIF-91 and ZIF-91-OLi using DFT calculation
(Red: oxygen, Blue: nitrogen, White: hydrogen and Gray: carbon; Color Map. Red: Negative, Blue: Positive)

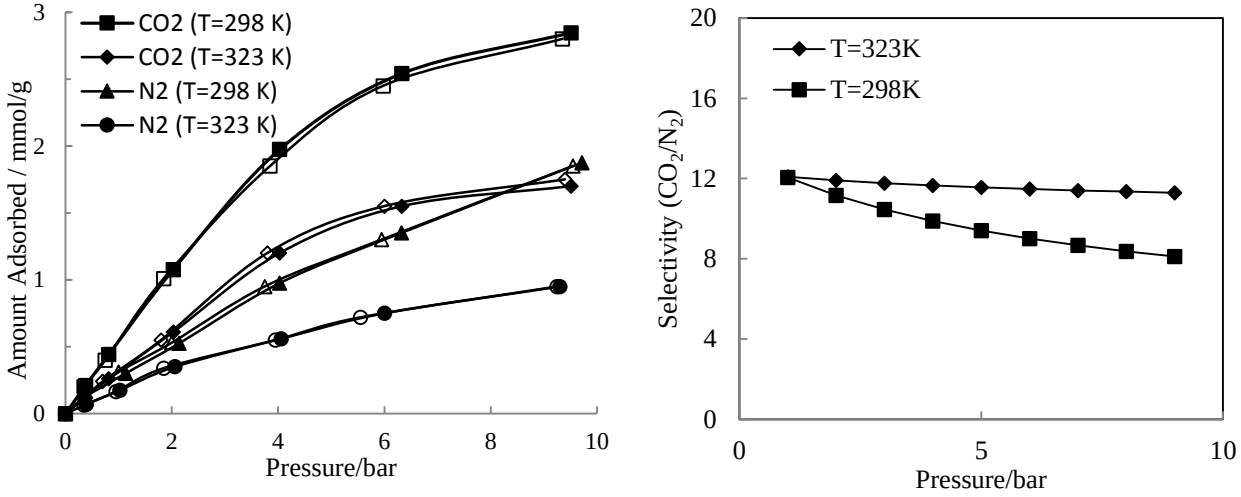

Fig. S5: Experimental adsorption isotherms of CO_2 and N_2 over the as-synthesized ZIF-91at 298 and 323 K (left) and calculated selectivity of CO_2/N_2 at corresponding temperatures (right)

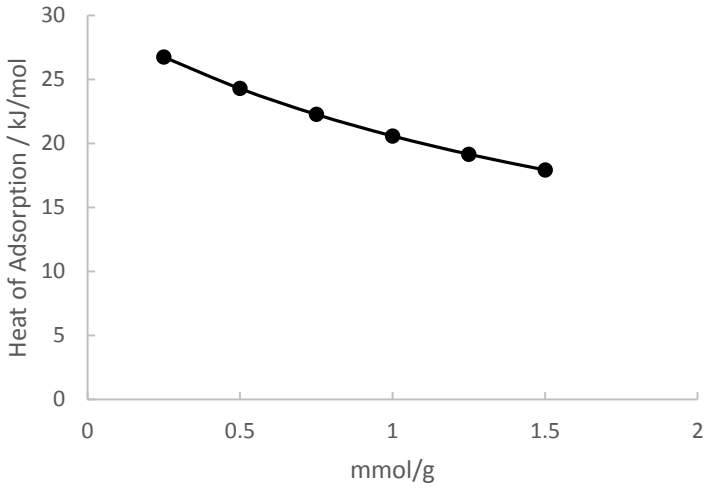

Fig. S6: Isosteric heat of adsorption for CO_2 over the ZIF-91

Table S1. The ICP analysis performance of ZIF-90-OLi structure to obtain the actual content of Li^+ in the structure

SPECTRO

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		Current User:	spectro
Method Name:	30MULTIELEMENT METHO	Creation Date:	2017-08-29 12:31:14
Method Autor:	spectro	Last Change:	2017-10-22 11:39:22

Sample Name: SAMPLE1-MS GHAHREMANI-1:10			Sample Type: Unknown Sample			
Measure Date: 2017-10-22 11:0	Recalc. Date:		State: Measured	Quality: Drifted	Total Dilution: 10.000000	
Sample Identification						
Sample Name	DILUTION	VOLUME	WEIGHT			
SAMPLE1-MS GH.	10.000000	25	0.0136			

	Li.						
Conc 1	6338.88[ppm]						
Conc 2	6235.46[ppm]						
Conc MinRange	---						
Conc Mean	**6287.17[ppm]**						
Conc MaxRange	---						
Reported	**6287.17[ppm]**						

Table S2. Textural properties of as-synthesized ZIF-90-OLi in comparison with ZIF-90 and ZIF-91

Sample	BET surface area (m^2/g)	Langmuir surface area (m^2/g)	Pore volume (cc/g)	Mean Pore Diameter (nm)
ZIF-90	717.96	779.90	0.6325	3.52
ZIF-91	266.80	272.74	0.4544	6.82
ZIF-91-OLi	523.12	576.23	0.3002	2.29