

Figure S1 ^1H NMR spectra of d-HKUST-1 digested in DCl/DMSO- d_6 mixture.

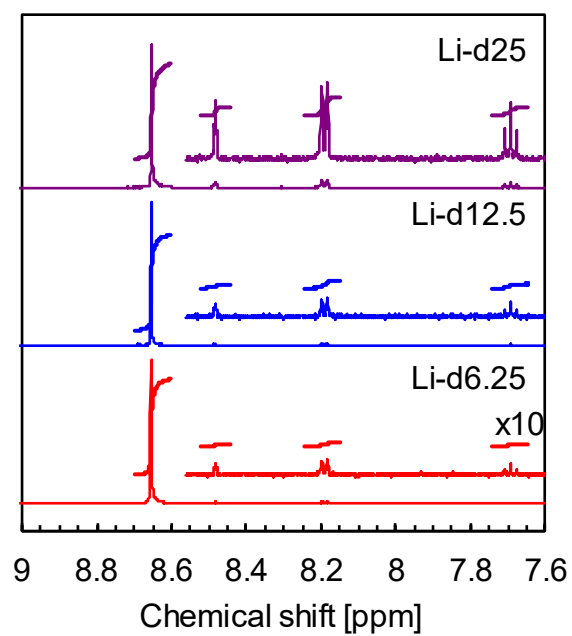


Figure S2 ^1H NMR spectra of Li-d-HKUST-1 digested in DCl/DMSO- d_6 mixture.

Table S1 Comparison of Li doping agent, Li/metal ratio, surface area, and H₂ uptake at 77 K and 1 bar for other Li-doped MOFs.

MOFs	Li agent	Li/metal [mol%]	BET surface area [m ² /g]	H ₂ uptake [wt%]	Ref.
HKUST-1	0	0	1705	2.37	This work
Li-10	Li(NO ₃) ₂	0.29	1548	2.37	This work
Li-20	Li(NO ₃) ₂	0.24	1706	2.47	This work
Li-200	Li(NO ₃) ₂	0.93	1251	1.94	This work
Li-d6.25	Li(NO ₃) ₂	0.64	1687	2.63	This work
Li-d12.5	Li(NO ₃) ₂	0.85	1544	3.03	This work
Li-d25	Li(NO ₃) ₂	0.51	1330	2.14	This work
Me ₂ NH ₂ [In(L ₁)] ^a	–	0	820	1.39	[33]
Li _{0.5} (H ₃ O) _{0.5} [In(L ₁)] ^a	LiCl	50	1024	1.66	[33]
[H ₂ ppz][In ₂ (L ₂) ₂] ^b	–		180	0.96	[16]
Li _{1.5} [H ₃ O] _{0.5} [In ₂ (L ₂) ₂] ^b	LiCl	75	580	1.02	[16]
Zn ₂ (NDC) ₂ (diPyTz)	–	0	400	1.12	[34]
Li · Zn ₂ (NDC) ₂ (diPyTz)	Li-Naph ^c	5	526	1.46	[34]
DO-MOF		0	810	1.23	[19]
DO-MOF-Li0.20	LiOtBu ^d	10	840	1.32	[19]
DO-MOF-Li2.62	LiOtBu ^d	262	270	0.77	[19]
HKUST-1	–	0	1587	2.41	[35]
Li-HKUST-1	Li-Naph ^c	7	795	3.50	[35]
MIL-101(Cr)	–	0	2537	2.37	[35]
Li-MIL-101(Cr)	Li-Naph ^c	1	1840	3.39	[35]
MIL-53(Al)	–		976	1.66	[15]
Li-MIL-53(Al)	Li(NO ₃) ₂	4	958	1.84	[15]
MOF-5-OH-0.38	–	0	3220	1.23	[17]
MOF-5-Oli	LDA ^e	19	3190	1.39	[17]
RHA-MIL-101	–	0	2525	1.54	[18]
0.06Li-RHA-MIL-101	Li(NO ₃) ₂	0.06 wt%	2942	2.65	[18]
0.3Li-RHA-MIL-101	Li(NO ₃) ₂	0.32 wt%	2141	2.42	[18]
0.6Li-RHA-MIL-101	Li(NO ₃) ₂	0.63 wt%	1825	1.69	[18]
6.0Li-RHA-MIL-101	Li(NO ₃) ₂	6.09 wt%	1073	1.58	[18]

^aH₄L₁ = biphenyl-3,3',5,5'-tetracarboxylic acid; ^bH₄L₂ = 1,1',4',1'',4'',1'''-quaterphenyl-3,5,3'',5'''-tetracarboxylic acid; ^cLi-Naph = lithium naphthalene; ^dLiOtBu = Lithium tert-Butoxide; ^eLDA = Lithium diisopropylamide

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