Online Supporting Information for

Computer-Aided Design of Interpenetrated Tetrahydrofuran-Functionalized 3D Covalent Organic Frameworks for CO_2 Capture

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Table S1. CO_2 uptake capacity in selected interpenetrated MOFs at 298 K and 1 atm in comparison with our designed COF.

Frameworks	*Degree of Interpenetration n-Fold*	*CO_2 uptake capacity, mmol/g*	*Reference*
PCN-124	self-interpenetrated	5.08	1
Cu-TATB-60	2-fold	4.29 (3.54)[b]	2
SUMOF-2	2-fold	4.26[a] (1.55)[b]	3
Cd-ANIC-1	2-fold	3.84	4
Co-ANIC-1	2-fold	3.48	4
PMOF-3	2-fold	3.24	5
UHM-6	2-fold	2.10	6
SNU-71'	2-fold	1.05 (0.79)[b]	7
MOF-508b	2-fold	1.80	8
$Zn_5(BTA)_6(TDA)_2$	4-fold	1.65	9
$Cu_2(HBTB)_2$	2-fold	1.30	10
YO-MOF	2-fold	1.20	11
NOTT-202[a]	partial-interpenetrated	1.20	12
UCY-1	2-fold	0.98	13
In-MOF1	2-fold	0.77	14
M'MOF-20	3-fold	0.45	15
COF_THF	4-fold	4.60	This work
COF_THF	5-fold	4.00	This work

[a] at 273K and 1 atm, [b] numbers in parentheses are for the non-interpenetrated framework.

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