

Supplementary Information

High hydrogen release by cryo-adsorption and compression on porous materials

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Table S1. Textural properties and excess H₂ uptakes at 77 K and 0.1 MPa of different HCPs reported in the literature.

Sample	Monomer or precursor	Synthetic strategy	$A_{\text{BET}}^{\text{a}}$ ($\text{m}^2 \text{g}^{-1}$)	$V_{\text{micro}}^{\text{b}}$ ($\text{cm}^3 \text{g}^{-1}$)	$V_{\text{TN}_2}^{\text{c}}$ ($\text{cm}^3 \text{g}^{-1}$)	Excess H ₂ uptake at 77 K and 0.1 MPa (wt.%)	Ref.
1	benzene	Friedel–Crafts catalysis with FeCl ₃	1391	0.48	2.42	1.45	1
1a	benzene		1270	0.43	1.67	1.32	
1B	benzene		897	0.31	0.70	1.01	
2	biphenyl		815	0.33	0.46	1.34	
2A	biphenyl		397	0.26	0.15	0.72	
2B	biphenyl		195	0.21	0.07	0.51	
3	1,3,5 triphenylbenzene		1059	0.44	0.71	1.58	
4	methylbenzene		826	0.31	0.53	1.05	
5	chlorobenzene		438	0.16	0.36	0.64	
1	poly(divinylbenzene-covinylbenzyl chloride) (DVB-VBC) precursors	Friedel–Crafts catalysis with FeCl ₃	1420	0.09	1.29	1.20	2
9			1520	0.39	0.82	1.45	
10			1430	0.27	0.77	1.43	
11			1370	0.39	0.70	1.43	
12			1260	0.39	0.63	1.42	
FCBCz	carbazoles, dicarbazole and tricarbazole	Friedel–Crafts catalysis with FeCl ₃	1067	0.43	0.71	1.56	3
FCTCz			1845	0.51	2.91	1.94	
C1M1	benzene/ biphenyl/1,3,5-triphenylbenzene	Friedel–Crafts catalysis with	688	0.19	0.40	0.80	4
C1M2-AI			1164	0.26	0.73	1.45	

C1M3-AL		FeCl ₃	1783	0.37	1.29	1.91	
MPNs	vinylbenzyl chloride (VBC)/divinylbenzene (DVB)	Emulsion polymerization	1500	0.44	1.71	1.59	5
Diiodomethane (6)	polyaniline and diiodoalkanes or paraformaldehyde	Friedel–Crafts catalysis with FeCl ₃	632	0.29	0.94	0.96	6
-	polyaminobenzenes or aniline with polyhalogenobenzenes or aniline with polyhalogenobenzenes	Ullman and Buchwald synthetic routes	316	0.13	0.25	0.85	7
PCz-C3-Cz	four carbazole-based conjugated networks PCz–C3–Cz to PCz–C6–Cz	Friedel–Crafts catalysis with FeCl ₃	862	0.34	0.54	1.21	8
PCz-C4-Cz			870	0.34	0.62	1.33	
PCz-C5-Cz			768	0.30	0.61	1.28	
PCz-C6-Cz			785	0.31	0.61	1.22	
HCP-BDM	BDM, BA, BC	Friedel–Crafts catalysed self-condensation	847	0.21	0.55	1.11	9
HCP-BA			742	0.14	0.51	0.97	
POPS-2	octaphenyl POSS	Friedel–Crafts and Scholl coupling reactions	472	0.11	0.28	0.89	10
POPS-1			795	0.13	0.59	0.89	

^a Brunauer-Emmett-Teller area.

^b Micropore volume (*i.e.*, volume of pores of width < 2nm).

^c Total pore volumes determined from the N₂ adsorption isotherm at P/P^o in the range 0.97-0.99.

Table S2. Textural properties and H₂ uptakes at 77 K and high pressure of different HCPs reported in the literature.

Sample	Monomer or precursor	Synthetic strategy	A_{BET}^a (m ² g ⁻¹)	V_{micro}^b (cm ³ g ⁻¹)	$V_{\text{TN}_2}^c$ (cm ³ g ⁻¹)	Excess H ₂ uptake 77 K and high pressure (wt.%)	Pressure of the measurement (MPa)	Type of uptake	Ref.
-	vinylbenzyl chloride	Friedel–Crafts catalyst with FeCl ₃	1466	0.48	-	3.04	1.5	absolute	11
UPO16	tetraphenylmethane (TPM)	Friedel–Crafts catalysis	1289	0.31	0.96	2.3	3	excess	12
Diiodomethane (6)	polyaniline and diiodoalkanes or paraformaldehyde	Friedel–Crafts catalysis with FeCl ₃	632	0.29	0.94	2.2	3.00	excess	6
SB-CO-PP-20	pyrrole and sugar beet leaves for the HCP and the AC, respectively	Oxidation with ammonium persulfate	1421	0.616	0.857	2.2	2	excess	13
SB-CO-PP-7	pyrrole and sugar beet leaves for the HCP and the AC, respectively	Oxidation with ammonium persulfate	820	0.355	0.932	1.6	2	excess	
SBL-PNP-0.25–2–600	pyrrole and sugar beet leaves for the HCP and the AC, respectively	Oxidation with ammonium persulfate	588	0.23	0.42	1.56	2	excess	14
SBL-PNP-0.5–2–600	pyrrole and sugar beet leaves for the HCP and the AC, respectively	Oxidation with ammonium persulfate	480	0.157	0.175	1.5	2	excess	
SBL-PNP-1–2–600	pyrrole and sugar beet leaves for the HCP and the AC, respectively	Oxidation with ammonium persulfate	380	0.11	0.13	1.77	2	excess	

27	bischloromethyl monomers	Self-condensation	1370	0.49	2.65	3.18	1.5	absolute	15
43	bischloromethyl monomers		1904	0.63	2.80	3.68	1.5	absolute	

^{a, b, c} have the same meaning as in Table S1.

Table S3. Textural properties and excess H₂ uptakes at 77 K and high pressure of different ACs from the open literature.

Sample	A_{BET}^a	$V_{\text{T N}_2}^b$	$V_{\text{DR N}_2}^c$	$V_{\text{DR CO}_2}^d$	Excess H ₂ uptake at 77 K and high pressure	Measurement pressure	Information	Ref.
	(m ² g ⁻¹)	(cm ³ g ⁻¹)	(cm ³ g ⁻¹)	(cm ³ g ⁻¹)	(wt.%)	(MPa)		
MSC30	3305	1.6	1.02	0.37	5.8	4	Commercial ACs	16
MSP20X	1737	0.93	0.37	0.42	4.8	4	Commercial ACs	
AC251	2082	0.89	0.72		5.4	4	AC doped with urea	17
M2029	2029	0.83	0.75	0.47	4.8	4	Anthracites-derived, chemically activated with KOH	18
T2275	2275	1.03	0.79	0.37	5.3	4		
T2502	2502	1.11	0.83	0.39	5.7	4		
M2849	2849	1.31	0.97	0.45	5.9	4		
T3073	3073	1.4	0.98	0.41	5.6	4		
M1149	1149	0.45	0.44	0.49	3.2	4		
T1308	1308	0.57	0.47	0.32	3.1	4		
T3220	3320	1.5	1.02	0.49	5.5	4		
A704	1535	-	-	0.55	3.2	4	Anthracites-derived, chemically activated with KOH	19
A754	1717	-	-	0.61	3.7	4		
A804	1746	-	-	0.61	3.5	4		
A753	1464	-	-	0.54	3.2	4		
A55	2018	-	-	0.68	3.9	4		
LaB753	1647	-	-	0.55	3.6	4	Low-ash Bituminous activated with KOH	
Ch800/700/3	2481	0.95	0.84	-	5	4	Chitosan-based, activated with KOH	20
Ch900/700/3	2192	0.93	0.87	-	4.6	4		
Ch1000/700/3	1638	0.7	0.67	-	3.62	4		
Ch900/800/1	922	0.4	0.37	-	2.5	4		
Ch700/700/3	3066	1.38	1.11	-	5.61	4		
AC-K5	3190	1.69	1.09	-	7.08	2	Commercial ACs activated with KOH	21
AC-K3	2009	1	0.82	-	5.63	2		
CA-4700	3800	1.75	1.54	-	7	2		22

KUA6	3808	-	1.27	0.68	5.6	4	Anthracites-derived, chemically activated with KOH	23
KUA5	3183	-	1.1	0.72	5.4	4		
AX21	2513	-	0.93	0.68	4.9	4	Commercial ACs	
H1	2122	-	0.92	0.89	4.0	4	-	
KUA4	1953	-	0.87	0.7	3.8	4	Anthracites-derived, chemically activated with KOH	
KUA3	1694	-	0.71	0.68	3.2	4		
KUA2	1330	-	0.58	0.54	2.9	4		
KUA1	1058	-	0.51	0.5	2.4	4		

^a Brunauer-Emmett-Teller area.

^b Total pore volumes determined from the N₂ adsorption isotherm at P/P^o in the range 0.97-0.99.

^c Micropore volume (< 2nm) calculated using the Dubinin-Raduskevich (DR) equation applied to the N₂ adsorption data.

^d Micropore volume (< 2nm) calculated using the Dubinin-Raduskevich (DR) equation applied to the CO₂ adsorption data.

Table S4. Textural properties and excess H₂ uptakes at 298 K and 2 MPa of different ACs from the open literature.

Sample	$A_{\text{BET}}^{\text{a}}$ ($\text{m}^2 \text{g}^{-1}$)	$V_{\text{T N}_2}^{\text{b}}$ ($\text{cm}^3 \text{g}^{-1}$)	$V_{\text{DR N}_2}^{\text{c}}$ ($\text{cm}^3 \text{g}^{-1}$)	Excess H ₂ uptake (wt.%)	Measurement pressure (MPa)	Description	Ref.
AcHTC 0,2 4	1422	0.64	0.52	0.16	2	Hydrochar- derived, chemically activated with KOH	24
AcHTC 0,4 1	692	0.31	0.26	0.08	2		
AcHTC 0,4 2	897	0.36	0.34	0.10	2		
AcHTC 0,4 3	1020	0.57	0.38	0.12	2		
AcHTC 0,4 4	2032	0.93	0.72	0.18	2		
AcHTC 0,4 5	2045	1.04	0.71	0.20	2		
AcHTC 0,8 3	1347	0.53	0.5	0.17	2		
AcHTC 0,8 4	1425	0.62	0.51	0.16	2		
AcHTC 0,8 5	2703	1.45	0.9	0.18	2		
AcHTC 1,6 3	1499	0.67	0.54	0.16	2		
AcHTC 1,6 5	2180	0.98	0.71	0.17	2		

^a Brunauer-Emmett-Teller area.

^b Total pore volumes determined from the N₂ adsorption isotherm at P/P° in the range 0.97-0.99.

^c Micropore volume (< 2 nm) calculated using the Dubinin-Raduskevich (DR) equation applied to the N₂ adsorption data.

Table S5. Textural properties and excess H₂ uptakes at 298 K and 5 MPa of different ACs from the open literature.

Sample	$A_{\text{BET}}^{\text{a}}$ (m ² g ⁻¹)	$V_{\text{T N}_2}^{\text{b}}$ (cm ³ g ⁻¹)	$V_{\text{DR N}_2}^{\text{c}}$ (cm ³ g ⁻¹)	$V_{\text{DR CO}_2}^{\text{d}}$ (cm ³ g ⁻¹)	Excess H ₂ uptake (wt.%)	Measurement pressure (MPa)	Description	Ref.
M2029	2029	0.83	0.75	0.47	0.5	5	Chemical activation of anthracites with alkali (Na and K) hydroxides	18
T2275	2275	1.03	0.79	0.37	0.5	5		
T2502	2502	1.11	0.83	0.39	0.5	5		
M2849	2849	1.31	0.97	0.45	0.6	5		
M1149	1149	0.45	0.44	0.49	0.4	5		
T1308	1308	0.57	0.47	0.32	0.4	5		
T3073	3073	1.4	0.98	0.41	0.6	5		
T3220	3220	1.5	1.02	0.49	0.6	5		
AcHTC 0,4 1	692	0.31	0.26	-	0.23	5.6	Hydrochar-derived, chemically activated with KOH	24
AcHTC 0,4 3	1020	0.57	0.38	-	0.32	5.5		
AcHTC 0,4 5	2045	1.04	0.71	-	0.39	5.5		
KUA5	3183	-	1.1	0.72	0.56	5.8	Anthracites-derived, chemically activated with KOH	23
AX21	2513	-	0.93	0.68	0.48	5.8	Commercial ACs	
KUA6	3808	-	1.27	0.68	0.46	5.8	Anthracites-derived, chemically activated with KOH	
Maxsorb	3178	-	1.2	0.69	0.46	6.1	Commercial ACs	
A20	1666	-	0.79	0.43	0.41	5.9		
KUA1	1058	-	0.51	0.5	0.31	5.9	Anthracites-derived chemical activated with KOH	

^{a, b, c, d} have the same meaning as in Table S3.

Table S6. Textural properties and excess H₂ uptakes at 298 K and 10 MPa of different ACs from the open literature.

Sample	$A_{\text{BET}}^{\text{a}}$ (m ² g ⁻¹)	$V_{\text{T N}_2}^{\text{b}}$ (cm ³ g ⁻¹)	$V_{\text{DR N}_2}^{\text{c}}$ (cm ³ g ⁻¹)	$V_{\text{DR CO}_2}^{\text{d}}$ (cm ³ g ⁻¹)	Excess H ₂ uptake (wt.%)	Pressure (MPa)	Description	Ref.
AcHTC 0,4 1	692	0.31	0.26	-	0.32	10	Hydrochar-derived, chemically activated with KOH	24
AcHTC 0,4 3	1020	0.57	0.38	-	0.46	10		
AcHTC 0,4 5	2045	1.04	0.71	-	0.54	10		
KUA5	3183	-	1.1	0.72	0.75	9	Anthracites-derived, chemically activated with KOH	23
AX21	2513	-	0.93	0.68	0.73	10		
KUA6	3808	-	1.27	0.68	0.71	10		
Maxsorb	3178	-	1.2	0.69	0.68	10		
A20	1666	-	0.79	0.43	0.54	9		
KUA1	1058	-	0.51	0.5	0.44	10		
KC-RS_3	2100	0.95			0.65	10	Rice-derived, activated with KOH	25

^{a, b, c, d} have the same meaning as in Table S3.

Table S7. Textural properties and excess H₂ uptakes at 298 K and 20 MPa of different ACs from the open literature.

Sample	$A_{\text{BET}}^{\text{a}}$	$V_{\text{T N}_2}^{\text{b}}$	$V_{\text{DR N}_2}^{\text{c}}$	$V_{\text{DR CO}_2}^{\text{d}}$	Excess H ₂ uptake	Pressure	Description	Ref.
	(m ² g ⁻¹)	(cm ³ g ⁻¹)	(cm ³ g ⁻¹)	(cm ³ g ⁻¹)	(wt.%)	(MPa)		
Anthracites-KOH_1073	2365	1.04	0.84		0.96	20	Anthracites-derived, chemically activated with KOH	26
Anthracites-KOH_1023	2087	0.89	0.76		0.88	20		
Anthracites-KOH_973	1929	0.83	0.71		0.83	20		
Anthracites-NaOH_1023	1722	0.73	0.62		0.80	20		
Anthracites-NaOH_973	1635	0.68	0.60		0.76			
KUA5	3183	-	1.27	0.68	1.16	20	Anthracites-derived, chemically activated with KOH	23
AX21	2513	-	0.93	0.68	1.14	20	Commercial ACs	
KUA6	3808	-	1.27	0.68	1.09	20	Anthracites-derived, chemically activated with KOH	
Maxsorb	3178		1.2	0.69	1.06	20	Commercial ACs	

^{a, b, c, d} have the same meaning as in Table S3.

Table S8. Textural properties and H₂ uptakes at 298 K and 35-42 MPa of different ACs from the open literature.

Sample	A_{BET}^a	$V_{\text{T N}_2}$^b	Excess H₂ uptake	Pressure	Description	Reference
	(m ² g ⁻¹)	(cm ³ g ⁻¹)	(wt.%)	(MPa)		
AX-21	2664	1.36	1.77	35		27
MSC30	3476	2.04	1.52	40		
KUA-5	2887	1.37	1.52	42	Anthracites-derived, chemically activated with KOH	

^a Brunauer-Emmett-Teller area.

^b Total pore volumes determined from the N₂ adsorption isotherm at P/P^o in the range 0.97-0.99.

Table S9. Textural properties and H₂ uptakes of different MOFs reported in the literature.

Sample	$\rho_{\text{crys}}^{\text{a}}$	$\rho_{\text{sk}}^{\text{b}}$	$\rho_{\text{TAP}}^{\text{c}}$	$V_{\text{T N}_2}^{\text{d}}$	L_0^{e}	$A_{\text{BET}}^{\text{f}}$	Excess H ₂ uptake ^g at 77 K	Measurement pressure	Absolute H ₂ uptake ^h at 77 K	Q_{st}^{i}
	g cm^{-3}	g cm^{-3}	g cm^{-3}	$\text{cm}^3 \text{g}^{-1}$	nm	$\text{m}^2 \text{g}^{-1}$	wt. %	MPa	wt. %	kJ mol^{-1}
DUT-6	0.386 ²⁸	1.66 ²⁸	0.23 ²⁸	2.02 ²⁸	1.2 ²⁸	4414 ²⁸	5.45 ²⁸	2.5	6.55 ²⁹	3.99 ²⁸
DUT-8(Co)	1.295 ^{28,30}	0.386 ²⁸	0.29 ²⁸	0.62 ²⁸	-	6632 ²⁸	1.15 ³⁰	2.5	1.31 ²⁹	4.55 ³⁰
DUT-9	0.467 ³¹	1.295 ^{28,30}	0.27 ²⁸	1.77 ³¹	-	3293 ³⁰	5.24 ³⁰	2.5	5.97 ²⁹	4.3 ³⁰
DUT-23(Co)	0.403 ²⁸	1.42 ²⁸	0.23 ²⁸	2.03 ³²	1.2 ²⁸	4850 ²⁸	6.73 ²⁸	2.5	7.61 ²⁹	3.93 ²⁸
MFU-4(Co)	1.179 ²⁹	1.93 ³⁰	0.44 ²⁸	-	0.9 ²⁸	1350 ³⁰	2.85 ³⁰	2.5	3.26 ²⁹	4.7 ³⁰
Mg-Formate	1.398 ²⁸	1.68 ²⁸	0.59 ²⁸	-	0.34 ²⁸	357 ³⁰	0.68 ²⁸	2.5	0.77 ²⁹	6.7 ²⁸
MIL-53 Fe	0.690 ²⁹	2.03 ²⁸	0.43 ²⁸	-	-	1677 ³⁰	2.71 ²⁸	2.5	3.11 ²⁸	5.6 ²⁸
Fe-BTCGel	-	1.81 ³⁰	0.69 ²⁸	-	-	772 ³⁰	1.62 ²⁸	2.5	1.86 ²⁹	5 ²⁸
MFU-4I	0.560 ³³	-	-	1.26 ³³	-	2750 ³³	4.00 ³³	2.5	4.35 ²⁹	3.50 ³³
MOF-5	0.605 ³⁴	-	-	1.37 ²⁹	1.2 ²⁸	2360 ³⁵	4.48 ³⁵	2.5	4.80 ²⁹	4.4 ³⁵
MIL-101(Cr)	0.610 ³⁶	-	-	1.85 ²⁸	0.7 ²⁸	2761 ²⁸	-	2.5	5.01 ²⁹	5.2 ²⁸
MOF-177	-	-	-	1.69 ³⁷	1.1 ³⁰	5250 ³⁷	6.28 ³⁰	2	6.92 ^a	3.7 ³⁰
HKUST-1	0.650 ³⁸	-	-	-	0.5 ²⁸	1527 ²⁸ / 1980 ³⁸	3.55 ²⁸	2	3.92 ^a	5.8 ²⁸
DUT-4	-	-	-	-	0.9 ²⁸	1308 ²⁸	2.13 ²⁸	2	2.08 ²⁹	5.35 ²⁹
DUT-5	-	-	-	-	1.1 ²⁸	1613 ²⁸	3.19 ²⁸	2	3.09 ²⁹	4.3 ²⁹
PAF-1	-	1.12 ³⁰	0.138 ³⁰	-	-	3363 ³⁰	5.97 ³⁰	2.5	-	4.2 ³⁰
NU-1101	0.459 ^{39,40}	-	-	2.82 ⁴¹	-	4340 ³⁹	5.7 ³⁹	3.76	7.66 ^a	5.5 ³⁹
NU-1102	0.40 ^{39,40}	-	-	-	-	3720 ³⁹	6.1 ³⁹	4.31	8.68 ^a	4.5 ³⁹
NU-1103	0.298 ^{39,40}	-	-	-	-	6245 ³⁹	7.0 ³⁹	4.88	11.01 ^a	3.8 ³⁹
NU-1501-Fe	0.299 ⁴²	-	-	2.9 ⁴²	1.5 ⁴²	7140 ⁴²	7.4 ⁴²	4	10.68 ^a	4 ⁴²
NU-1501-Al	0.283 ⁴²	-	-	2.91 ⁴²	1.5 ⁴²	7310 ⁴²	8.1 ⁴²	3.2	10.77 ^a	4 ⁴²
NU-1500-Al	0.498 ⁴²	-	-	1.46 ⁴²	1.4 ⁴²	3560 ⁴²	5.6 ⁴²	4	7.33 ^a	4.9 ⁴²
NU-100	0.290 ⁴¹	-	-	2.82 ⁴²	-	6143 ⁴²	9.05 ⁴¹	7	13.43 ^a	-
PCN-61	-	-	-	-	-	3000 ⁴³	5.9 ⁴³	3.3	-	6.36 ⁴³
PCN-66	-	-	-	-	-	4000 ⁴³	6.2 ⁴³	4.5	-	6.22 ⁴³

PCN-68	-	-	-	-	-	5109 ⁴³	6.8 ⁴³	5	-	6.09 ⁴³
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^a Samples' crystal density obtained by XRD.

^b MOFs' skeleton density obtained by He pycnometry.

^c MOFs' tapped density.

^d Total pore volumes determined from the N₂ adsorption isotherm at P/P^o in the range 0.97-0.99.

^e Average pore size.

^f Brunauer-Emmett-Teller area.

^g Excess uptake [wt.%] of H₂ calculated according to: $wt\% = \frac{\text{mass of H}_2}{\text{mass of H}_2 + \text{mass of MOF}} \times 100\%$.

^h Absolute uptake, calculated from the excess data using REPROF software to calculate the density of H₂ gas and considering the volume of the adsorbed phase volume to be equal to V_{T N₂}. The absolute uptake [wt.%] of H₂ was calculated according to:

$$wt\% = \frac{\text{mass of H}_2}{\text{mass of H}_2 + \text{mass of MOF}} \times 100\%$$

ⁱ Isotheric heat of H₂ adsorption.

Table S10. Absolute H₂ uptakes of different MOFs reported in the literature. The absolute uptake from the excess reported data was calculated using REPROF software to calculate the density of H₂ gas and considering the volume of the adsorbed phase to be equal to V_{pore} .

Sample	Pressure (MPa)	Gravimetric absolute H ₂ uptake at 77 K (mg g ⁻¹)	Volumetric absolute H ₂ uptake at 77 K (calculated from ρ_{crys}) (g cm ⁻³)	Ref.
DUT-6	2.5	70.1	27.1	29
DUT-8(Co)	2.5	13.3	17.2	
DUT-9	2.5	63.5	29.7	
DUT-23(Co)	2.5	82.4	33.2	
MFU-4(Co)	2.5	33.7	39.7	
Mg-Formate	2.5	7.8	10.9	
MIL-53 Fe	2.5	32.1	22.1	
Fe-BTCGel	2.5	19.0	0.0	
MFU-4I	2.5	45.5	25.5	
MOF-5	2.5	50.4	30.5	
MIL-101(Cr)	2.5	52.7	32.1	
MOF-177	2	74.4	32.0	
HKUST-1	2	40.8	26.5	28
DUT-4	2	21.3	-	
DUT-5	2	31.9	-	
NU-1101	3.76	83.0	38.1	39
NU-1102	4.31	95.1	38.3	
NU-1103	4.88	123.8	36.9	
NU-1501-Fe	4	119.6	35.8	42
NU-1501-Al	3.2	120.7	34.2	
NU-1500-Al	4	79.1	39.4	
NU-100	7	155.1	45.0	41

Table S11. Parameters of the modified Dubinin-Astakhov (MDA) ⁴⁴⁻⁴⁶ equation employed for calculating n_{exc} at specific temperatures and pressures. The parameters are valid over the employed range of cryogenic temperatures (77-160 K) and moderate pressures (0.5-10 MPa) for calculating the H₂ release capacity from 10 to 0.5 MPa.

Sample	m^a	V_a^b (cm ³ g ⁻¹)	n_{max}^c (mol kg ⁻¹)	α^d (J mol ⁻¹)	β^e (J mol ⁻¹ K ⁻¹)	P_0^f (MPa)	ρ_{sk}^g (g cm ⁻³)	P_{TAP}^h (g cm ⁻³)	V_{TN2}^i (g cm ⁻³)	Ref.	$\Delta n_{H_2}^j$ (at 77 K) (wt.%)	$\Delta n_{H_2}^k$ (from 77 K to 160K) (wt.%)
MSC30	2	1.5	72.5	3300	15.8	1013	2.51	0.25	1.6	¹⁶	10.0	13.2
MSP20X	2	1.09	47.4	4094	11.5	632	2.39	0.35	0.93		6.9	9.2
MOF-5	2	1.94	88.1	2403	11.50	322	2	0.30	-	^{47,48}	9.3	12.0

^a Exponent related to the heterogeneity of the material.

^b Parameter related to the adsorbed phase.

^c Parameter related to the saturation of the entire available pore volume.

^d Parameter related to the enthalpy of adsorption.

^e Parameter related to the entropy of adsorption.

^f Parameter related to the pseudo-saturation pressure according to Dubinin's definition.

^g Skeleton density obtained by He pycnometry.

^h Tapped density.

ⁱ Total pore volumes determinate from the N₂ adsorption isotherm at p/p^o in a range of 0.97-0.99.

^j H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 77 K.

^k H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 160 K.

The MDA parameters were used to determine n_{exc} as follows:

$$n_{exc} = n_{max} \exp \left[- \left(\frac{RT}{\alpha + T\beta} \right)^m \ln^m \left(\frac{P_0}{P} \right) \right] - \rho_g V_a \quad (S1)$$

where n_{exc} [mol kg⁻¹] is the excess hydrogen uptake, n_{max} [mol kg⁻¹] is the adsorbed hydrogen uptake equivalent to the saturation of the entire available pore volume, R [8.314 J mol⁻¹ K⁻¹] is the universal gas constant, α [J mol⁻¹] is the "enthalpy" factor, β [mol J⁻¹ K⁻¹] is the "entropy" factor ⁴⁶, P_0 [MPa] is the pseudo-saturation

pressure according to Dubinin's definition ⁴⁹, P [MPa] is the systems pressure, ρ_g [mol m⁻³], V_a [m³ kg⁻¹] is the volume of the adsorbed phase, and m is an exponent related to the heterogeneity of the material.

Using n_{exc} , we determined the total uptake, n_{tot} , as:

$$n_{tot} = n_{exc} + \rho_g (V_v) \quad (S2)$$

The void volume V_v was determined by Eq. (S3) ^{30,46}, where ρ_{TAP} [kg m⁻³] is the tapped density, and ρ_{sk} [kg m⁻³] is the crystal density.

$$v_v = \frac{1}{\rho_{TAP}} - \frac{1}{\rho_{sk}} \quad (S3)$$

The H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 77 K ($\Delta n_{H_2}^{77K \rightarrow 77K}$) and from 10 MPa and 77 K to 0.5 MPa and 160 K ($\Delta n_{H_2}^{77K \rightarrow 160K}$) were calculated from n_{tot} by Eq. (S3), where $n_{tot}^{max P}$ [mol kg⁻¹] is the total hydrogen uptake at the maximum tank pressure and $n_{tot}^{back P}$ [mol kg⁻¹] is the total hydrogen uptake at the minimum back pressure for a fuel cell.

$$\Delta n_{h_2} = n_{tot}^{max P} - n_{tot}^{back P} \quad (S4)$$

Table S12. H₂ release capacities of different MOFs reported in the open literature.

MOFs	$A_{\text{BET}}^{\text{a}}$ (m ² g ⁻¹)	$V_{\text{TN}_2}^{\text{b}}$ (cm ³ g ⁻¹)	$\rho_{\text{crys}}^{\text{c}}$ (g cm ⁻³)	Δn_{H_2} (77 K/10 MPa → 77 K/0.5 MPa) (from ρ_{crys})		Δn_{H_2} (77 K/10 MPa → 160 K/0.5 MPa) ^e (from ρ_{crys})		Ref.	
				(wt.%) ^d	(mg cm ⁻³) ^e	(wt.%) ^f	(mg cm ⁻³) ^g		
NU-1101	4340	1.72	0.459	6.1	31	9.1	47	39	
NU-1102	3720	1.65	0.403	6.9	31	9.6	44		
NU-1103	6245	2.72	0.298	10.1	33	12.6	43		
NU-1500-Al	3560	1.46	0.498			8.2	44.6	42	
NU-1501-Fe	7140	2.9	0.299			13.2	45.6		
NU-1501-Al	7310	2.91	0.283			14	46.2		
MOF-5	3510	1.36	0.59			7.8	51.9	50	
NU-100	6050	3.17	0.29			13.9	47.6	38	
HKUST-1	1980	0.75	0.881	2	17	4.9	46		
IRMOF-20	4070	1.65	0.51			9.1	51		
TT-112	3440	1.44	0.446	5.3	24	8.3	41		
NU-125	3230	1.33	0.578	4.1	24	7.8	49		
rht-MOF-7	1950	0.79	0.789	1.8	14	4.5	37		
Cu-MOF-74	1270	0.47	1.323	1	13	2.9	39		
PCN-250	1780	0.71	0.896	1.8	16	4.9	47		
NU-1000	2200	1.48	0.571	5.2	30	7.7	48		
UiO-67	2360	0.91	0.688	2.9	20	5.7	41		
UiO-68-Ant	3030	1.17	0.607	4.3	26	7.2	47		
CYCU-3-Al	2450	1.56	0.477	5.5	27	8	41		
SNU-70	4940	2.14	0.411			10.6	47.9		51
UMCM-9	5040	2.31	0.37			11.3	47.4		

^a Brunauer-Emmett-Teller area.

^b Total pore volumes determined from the N₂ adsorption isotherm at P/P^o in the range 0.97-0.99.

^c Samples' crystal density obtained by XRD.

^d H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 77 K in gravimetric basis [wt.%], calculated as: $\text{wt}\% = \frac{\text{mass of H}_2}{\text{mass of H}_2 + \text{mass of MOF}} \times 100\%$.

^e H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 77 K in volumetric basis, calculated using ρ_{crys} .

^f H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 160 K in gravimetric basis [wt.%] calculated as $\text{wt}\% = \frac{\text{mass of H}_2}{\text{mass of H}_2 + \text{mass of MOF}} \times 100\%$.

^g H₂ release capacity from 10 MPa and 77 K to 0.5 MPa and 160 K in volumetric basis, calculated using ρ_{crys} .

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