The application of amine-based materials for carbon capture and utilisation: an overarching view

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Table S1. Performance of various selected polyamine-based CO_2 adsorbents (under flue gas or air –relevant conditions).

Adsorbent (class)	Amine (wt% / mmol N/g)	Temp. / °C (des. gas)	CO2 conc.[a] (humidity)	Total system pressure[b]	CO2 capacity[c] / mmol/g	Method	No. cycles	Comments	Ref.
INORGANIC OXIDE-SUPPORTED									
48% PEI/SBA-15	PEI (M_w 1800) 48 wt% (11.14 mmol N/g)	Ads: 30 Des: 120	400 ppm	1 atm	1.10	TGA			(1)
41% PEI/SBA-15	PEI (M_w 1800) 48 wt% (9.52 mmol N/g)	Ads: 30 Des: 120	10%	1 atm	1.23	TGA			(1)
50% PPG/SBA-15 (1)	PPG (50 wt%)	Ads: 30 Des: 120	400 ppm	1 atm	0.63	TGA			(1)
	PPG (50 wt%)	Ads: 30 Des: 120	10%	1 atm	1.12 – 0.49	TGA	5		(1)
EtSNTs-50 PEI encapsulated in nanotubes	PEI (Mw 600) (11.2 mmol N/g)	Ads: 30 Des: 100	400 ppm	1 atm	~ 1.00	Fix bed Reactor (breakthrough)	8		(2)

40% TPTA/SBA-15	TPTA 41 wt% organic (8.71 mmol N/g)	Ads: 35 Des: 70	400 ppm	1 atm	3.15 mmol CO2/g SiO2 (1.86 mmol/g sorbent)	TGA			(3)
SBA-15/PEI/PEG200	PEI (Mw 800) (8.38 mmol N/g)	Ads: 30 Des: 110	400 ppm	1 atm	1.64	TGA			(4)
Templated Alumina/PEI/PEG200	PEI (Mw 800) (5.98 mmol N/g)	Ads: 30 Des: 110	400 ppm	1 atm	1.29	TGA			(4)
TRI-SBA-15-130-0.4 (2)	TRI (~30 wt% organic)	Ads: 25 Des: 120 (N_2)	5%	1 atm	1.88	TGA			(5)
		Ads: 25 Des: 120 (N_2)	5%	1 atm	1.78 − 1.82	TGA	12		(5)
(PEI-25-APTES-25)-PQCS2129 (1/2)	PEI, APTES (7.5 mmol N/g)	Ads: 40 Des: 120 (N_2)	0.04 bar	0.81 bar	2.70	Perkin−Elmer Pyris 1 TGA		N_2 to balance pressure during adsorption. Isosteric heat of adsorption at CO_2 uptake of 2.6 mmol/g calculated as 56 kJ/mol CO_2.	(6)
		Ads: 60 Des: 105 (He) Regen:105 (He, 90 vol % H_2O)	10% (8 vol %)	1.01 bar	2.43 ± 0.26	Fixed-bed flow system (breakthrough)	8	Regeneration under highly humidified He stream.	(6)
PEI / TMPED / silica (1/2)	PEI, TMPED	Ads: 50 Des: 175 (He/ N_2, 4% v/v H_2O)	13.4% (4% v/v)	1 atm	1.80 − 2.00	Fixed bed reactor	>100		(7)
FS-PEI-50 (1)	PEI (M_w 25,000) (50 wt %)	Ads: 25 Des: 85 (0.9 x10^{-3} bar) Regen:(air)	Ambient air (410 – 420 ppm)	10.3 bar	1.65 – 1.71	All-glass, grease-free flow system (Breakthrough)	4	"Air from the laboratory atmosphere was dried filtered and compressed to 150 psi and used directly for the	(8)

								adsorption measurements”	
		Ads: 25 Des: 85 (0.9 x10^{-3} bar)	Ambient air (410 – 420) ppm (RH 67%)	10.3 bar	1.41				(8)
FS-PEI-33 (1)	PEI (M_w 25000) (33 wt %)	Ads: 25 Des: 85 (0.9 x10^{-3} bar)	Ambient air (410 – 420 ppm) (RH 67%)	10.3 bar	1.74				(8)
PEHAS13 – MCF support (3)	PEI/aziridine (4.49 mmol N/g)	Ads: 75 Des: 110 (Ar)	10% (100% water saturation)	1 atm	0.85	packed bed flow reactor (Breakthrough)		Adsorption experiments were ended when the uptake rates became less than 0.2 µmol CO_2/min.	(9)
S-70C-2-24h (3)	PEI/aziridine (7.23 mmol N/g) SBA-15 Mesoporous Silica	Ads: 25 Des: 110	10%	1 atm	0.93	TGA			(10)
SynA50 (1)	PEI (M_w 800) (11.20 mmol N/g) γ-alumina	Ads: 25 Des: 110 (in Ar)	400 ppm	1 atm	1.74	TGA			(11)
		Ads: 25 Des: 110 (in Ar)	10%	1 atm	1.95	TGA			
SynA40 (1)	PEI (M_w 800) (8.66 mmol n/g) γ-alumina	Ads: 25 Des: 110 (in Ar)	400 ppm	1 atm	1.33	TGA			(11)
		Ads: 25 Des: 110 (in Ar)	10%	1 atm	1.73	TGA			
MS40 (1)	PEI (M_w 800) (9.23 mmol N/g) Mesoporous silica SBA-15	Ads: 25 Des: 110 (in Ar)	400 ppm	1 atm	1.05	TGA			(11)

		Ads: 25 Des: 110 (in Ar)	10%	1 atm	1.61	TGA			
PEI_H-SiO_2 (1)	PEI (M_w 800) 2.62 g PEI/g sorbent	Ads: 30 Des: 110 (He)	400 ppm (19% RH)	1 atm	3.36 − ~ 2.8	Fixed bed system (breakthrough)	5	The breakthrough measurement continued until the effluent CO_2 concentration reached 99 % of that of the feed stream.	(12)
		Ads: 30 Des: 110 (He)	400 ppm	1 atm	~ 2.34	Fixed bed system (breakthrough)	5		
		Ads: 50 Des: 110 (He)	400 ppm	1 atm	2.60	TGA			
		Ads: 80 Des: 110 (He)	10 %	1 atm	4.10	TGA			
PEI/Silica (1)	PEI (M_w 800) (10.5 mmol N/g)	Ads: 25 Des: 110	400 ppm	1 atm	2.36 − 1.65	TGA	4		(13)
A-PEI/Silica (1/2)	PEI (M_w 800), APTES (10.7 mmol N/g)	Ads: 25 Des: 110	400 ppm	1 atm	2.26 − 2.05	TGA	4		(13)
T-PEI/Silica (1)	PEI (M_w 800), tetrapropyl orthotitanate (10.5 mmol N/g)	Ads: 25 Des: 110	400 ppm	1 atm	2.19 − 2.16	TGA	4		(13)
PAA_MCM_41 (1)	PAA (M_n 1130 Da) (7.24 mmol N/g)	Ads: 25 Des: 120 (Ar)	400 ppm	1 atm	0.86	TGA			(14)
		Ads: 25 Des: 120 (Ar)	10%	1 atm	~ 1.50	TGA	3		

PEHA-PO-1-2/50S (1)	PEHA (59.5 wt% organic) 1:2 molar ratio of PEHA/propylene oxide	Ads: 25 Des: 60 (N_2)	400 ppm	1 atm	~ 1.25	TGA	15		(15)
TEPA-PO-1-2/50S (1)	TEPA (61.0 wt% organic) 1:2 molar ratio TEPA/propylene oxide	Ads: 25 Des: 60 (N_2)	400 ppm	1 atm	~ 1.34	TGA	15		(15)
OTHER SUPPORTED									
F-C-PSI, 10% PEI	PEI (M_w 800 Da) (5.2 mmol N/g fibre)	Ads: 37 Des: 110 (N_2)	10 mol% (100% RH)	1 atm	1.25 mmol/g fibre	Simulated flue gas flow system (breakthrough)		Capacity /g fibre	(16)
PAI/silica/PEI fibres	PEI (M_w 800) (5.9 mmol N/g fibre)	Ads: 35 Des: 90 (N_2)	14 mol% (100% RH)	1 atm	0.85 mmol/g fibre (b) 1.19 mmol/g fibre (q)	Simulated flue gas flow system (breakthrough)		Capacity /g fibre	(17)
		Ads: 35 Des: 120 (He)	10%	1 atm	1.02 − 0.83 mmol/g fibre	TGA	5	Capacity /g fibre	
PAI/silica/PEI fibres + glycerol	PEI (M_w 800) (5.9 mmol N/g fibre)	Ads: 35 Des: 90 (N_2)	14 mol% (100% RH)	1 atm	1.3 mmol/g fibre (b) 2.0 mmol/g fibre (q)	Simulated flue gas flow system (breakthrough)		Capacity /g fibre	(17)
PEI-CA-SiO_2	PEI (M_w 800 Da) 0.7 g PEI/g SiO2	Ads: 35 Des: 90 (N_2)	380 ppm	1 atm	0.62 mmol/g fibre (b) @ 95% of C0	Column breakthrough		Demonstrated vacuum-assisted desorption in TSA	(18)
		Ads: 35 Des: 110 (He)	395 ppm	1 atm	~0.62 mmol/g fibre	TGA	11	~95% of the CO_2 capacity was retained at the end of cycles	

PG-R20:1 PEI/glass fiber matrix + epichlorohydrin	PEI	Ads: 30 Des: 80 (vacuum)	16%	1 atm	0.26	Agilent 6820 gas chromatogram adsorption/desorption process (Breakthrough)			(19)
		Ads: 30 Des: 80 (vacuum)	16% (80% RH)	1 atm	3.98	(Breakthrough)			
PEI/G-silica sheets	PEI (M_n 600)	Ads: 75 Des: 120	15%	1 bar	3.89	magnetic suspension microbalance operated in a closed system	20		(20)
exfGO-D x 7.0TETA	TETA (7 g TETA/g sample = 88 wt%)	Ads: 75 Des: 70	100%	0.15 bar	7.5	Quantachrome Autosorb-iQC.			(21)
exfGO-D x 6.0TEPA	TETA (6 g/g sample = 86 wt%)	Ads: 75 Des: 100 (N_2)	15%	1 bar	6.4 − 5.0	TGA	50		(21)
HP20/PEI-50	PEI (50 wt %)	Ads: 25 Des: 100 (N_2)	400 ppm	1 atm	2.26 − 2.22	U-shaped glass tube	5		(22)
		Ads: 75 Des: 100 (N_2)	15 %	1 atm	2.95 − 2.91	TGA	5		
PEI/PIM-1 composite	PEI (M_w 800) (21 wt %)	Ads: 35 Des: 110 (vacuum < 5 mTorr)	100%	0.0004 bar	0.23	Micromeritics ASAP 2020			(23)
		Ads: 35 Des: 110 (vacuum < 5 mTorr)	100%	0.1 bar	1.15	Micromeritics ASAP 2020			
		Ads: 35 Des: 110	10%	1 atm	~0.9	TGA	10	Lost ~ 10% uptake capacity over 10 cycles	

		(N_2)							
A-PEI-300	PEI (M_w 300)	Ads: 25 Des: 110 (vacuum)	100%	0.15 bar	3.60	Volumetric (PCTpro-E&E)		Selectivity measurement showed no N_2 adsorption. IAST measured: from 12 - 45 kJmol/g between ~ 0.5 - 3.0 mmol CO_2/g	(24)
35 wt% PEI/3 wt% (Zn)ZIF-8/SiO2	PEI (M_w 800) 35 wt%	Ads: 50 Des: 120 (5.6 v/v% H_2O/N_2)	15% (5.6 v/v %)	1 atm	2.84 (50th cycle) (deactivation of 8% between 10 - 250th cycle)	Packed Bed Reactor	250	Adsorption gas included 4.5% O_2 Stability to SO_2, NO_x and H_2S measured	(25)
AEAPDMS-NFC	AEAPDMS-NFC (5.9 mmol N/g)	Ads: 30 Des: 90 (30 mbar)	400−530 ppm (60% RH)	1 atm	(average ads capacity) 0.90 reduction in adsorption capacity by up to 5%	Packed bed	100	TVS cycles, reduction of adsorption capacity by up to 5%.	(26)
PP-AM-HBP-NH2	PEHA (6.39 mmol N/g)	Ads: 25 Des: 90 (N_2)	10% volume	1 atm	5.60 ± 0.1	Breakthrough	15	Sample pre-swollen in water at 25 °C. Swelling degree was 81.69%.	(27)
UNSUPPORTED									
PEI-C60	PEI (M_w 25,000) (75 wt%)	Ads: 90 Des: 90 (vacuum)	100%	0.15 bar	3.41	Setaram PCTPro volumetric apparatus, (single component)		High CO_2/N_2 and CO_2/CH_4 selectivity demonstrated. Cycles showed 60% starting capacity after 100 cycles	(28)
PEI HB–4.0% EPC	PEI	Ads: ambient Des: 160 (air)	15%	~ 2 bar	~1.37	CO_2 filled balloon equipped with needle inserted into screw-cap septum seal of vial containing sample	10	Water weight ratio of sample 70% Sample also regenerated in microwave	(29)
1-G0/600PEI	PEI (M_w 600)	Ads: 25 Des: 120 (He)	60 mL/min CO_2/30 mL/min He	1 atm	0.93	TGA		Heat of adsorption 103 kJ mol/g at low adsorption values.	(30)

								Measured on Micromeritics ASAP-2020 apparatus	
		Ads: 65 Des: 120 (humid N_2)	15% (5.7 vol% H_2O)	1 atm	2.98 (average)	Packed bed reactor (breakthrough)	350	Simulated flue gas contained 4.5 vol% O_2	
1-G0-TEPA	TEPA (14 wt% N)	Ads: 25 Des: 120 (He)	60 mL/min CO2/30 mL/min He	1 atm	2.02	TGA			(31)
		Ads: 65 Des: 120 (humid N_2)	15% (5.7 vol% H_2O)	1 atm	1.68 (average)	Packed bed reactor (breakthrough)	25	Simulated flue gas contained 4.5 vol% O_2	
BC40	PEI (M_w 25,000) (5.79 mmol N/g)	Ads: 90 Des: 155 (100% CO_2)	10%	1 atm	2.16 − 2.14	TGA	29		(32)
		Ads: 90 Des: 110 (vacuum)	100%	0.1 bar	2.29	Isorb (Gas sorption analyzer)			
E200-FZ	PEI (M_w 750,000) (8.2 mmol N/g)	Ads: 25 Des: 110 (He)	10%	1 atm	2.01	TGA			(33)
		Ads: 25 Des: 110 (N_2)	10% (65% RH)	1 atm	3.36	Breakthrough			
E200-LN2	PEI (M_w 750,000) (8.8 mmol N/g)	Ads: 25 Des: 110 (He)	10%	1 atm	2.81	TGA			(33)
		Ads: 25 Des: 110 (N_2)	10% (65% RH)	1 atm	5.50	Breakthrough			

[a] If total pressure 1 atm, balance is inert gas Ar, He or N_2
[b] Total pressure assumed 1 atm unless otherwise stated for TGA and breakthrough
[c] Maximum adsorption capacity reported/equilibrium capacity
(b) breakthrough capacity
(q) pseudo equilibrium capacity

PEI: Polyethylenimine
PPG: Poly(propylene guanidine)
PAA: Poly(allylamine)
TEPA: Tetraethylenepentamine
TETA: Triethylenetetramine
PEHA: Pentaethylenehexamine
TRI: 3-[2-(2-Aminoethylamino)ethylamino]propyl trimethoxysilane
APTES: 3-(aminopropyl)triethoxysilane
TMPED: N^1-(3-trimethoxysilylpropyl)diethylenediamine
AEAPDMS-NFC: N-(2-aminoethyl)-3-aminopropylmethyldimethoxysilane nanofibrilated cellulose

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