Electronic Supplementary Material (ESI) for Materials Horizons.

Supporting Information

Porous Organic Polymers (POPs) for Environmental Remediation

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Table S1: Table of POPs-based materials for sensing of explosives.

POPs	Explosives	K_{sv} (M^{-1})	LOD	Mechanism	References
PNT-4	TNP	621901	2.36 nM	Absorption competition	1
PNT-5		507800	3.12 nM		
PNT-6		238278	5.52 nM		
COP-3	TNP	14533	<1 ppm	Static quenching & electron transfer	2
COP-4		3926	<1 ppm		
COP-401	TNP	8.3×10^4	<1 ppm	Electron transfer	3
COP-301		2.6×10^5	<1 ppm		
Py-azo-COP	TNP	1.37×10^3	--	Static quenching	4
CMP-LS1	TNP	5.05×10^4	--	Electron transfer; energy transfer	5
CMP-LS2		3.70×10^4	--		
PP_C-PPy_S-PAF	TNT	2.21×10^{-2} ppm^{-1}	--	Electron transfer	6
	TNP	2.42×10^{-2} ppm^{-1}	--		
TRIPTA	TNP	2.7×10^6	<51.96 nM	Static quenching	7
	DNP	2.13×10^6	--	Dynamic quenching	
	2,4-DNT	1.19×10^6	--	Dynamic quenching	
COP-61	TNP	2.40×10^5	<1 ppm	Electron transfer	8
COP-612	TNP	2.51×10^5	--	Static quenching	9
iPrTAPB-Azo-COP	TNP	1.1×10^4	--	Static quenching	10
PTPETCz	TNT	--	10 ppb	Electron transfer	11
PTPETPOcCz	TNT	--	1 ppm	Energy transfer	12
PHCPN	TNT	1.38×10^3	10 µM	--	13
LPCMP2	TNT	4147	3.64 µM	Electron transfer	14
FCMP3	2,4-DNT	5241	--	Charge transfer	15
	NB	2541	--		
	NT	4708	--		
TCB-CMP	2,4-DNT	5.9×10^3	--	Electron transfer	16
DTF	TNP	2.08×10^3	0.72 µM	--	17
TTPT	o-NP	6.20×10^3	2.18 nM	Electron transfer	18
TPV	RDX	--	~2-3 ag	Electron transfer	19
3'PD	TATP	3.03×10^4	--	Oxidation	20
	PA	1.0×10^5	--	Charge transfer	

Table S2: Table of POPs-based materials for sensing of cations.

POPs	Metal ions	K_{sv} (M^{-1})	LOD	Mechanism	References
HPP-3	Cu^{2+}	12785	--	Electron transfer	21
HLPPs	Cu^{2+}	400	--	Electron transfer	22
LMOP-15	Cu^{2+}	1.9×10^5	51 nM	Chelation & charge transfer	23
TSA-POPs	Cu^{2+}	--	--	Charge transfer	24
Salen-COP	Cu^{2+}	--	0.140 µM	Chelation & electron transfer	25
COP-108-S	Hg^{2+}	4.87×10^3	--	Electron transfer & static quenching	26

TNPP	Hg^{2+}	378450	22.8 ppb	Chelation & electron transfer	27
NOP-28	Hg^{2+}	3.7 x 10^4	12.0 ppb	Energy & electron transfer	28
CTFQD	Hg^{2+}	--	0.23 nM	Coordination	29
Cz-TPM@I	Hg^{2+}	--	4.9 µM	Charge transfer	30
PAF-5CF	Fe^{3+}	11865	38 µM	Absorption competition	31
DPA-CTF	Fe^{3+}	1.35 x 10^4	5.8 µM	Absorption competition	32
COP-100	Fe^{3+}	2.97 x 10^4	0.213 µM	Dynamic quenching	33
COP-401-COOH	Fe^{3+}	84682	--	Electron transfer	34
COP-401-SO_2Cl	Fe^{3+}	46106	--		
PNT-2	Fe^{3+}	20186	31 µM	Absorption competition	35
PNT-3	Fe^{3+}	23982	50.7 µM		
TPA-COP	Fe^{3+}	--	0.43 µM	Chelation	36
HLPPs	Fe^{3+}	8900	--	Electron transfer	37
POP-HT	Fe^{3+}	--	5 ppm	Lewis acid–base interaction	38
CMPAO	UO_2^{2+}	--	1.7 nM	Energy transfer	39
Salen-COP	Al^{3+}	--	0.248 µM	Electron transfer	40
Azo-Py	Al^{3+}	152	--	Electrostatic attraction	41
COP-100	Fe^{2+}	2.58 x 10^4	0.245 µM	Dynamic quenching	42
TPBCz-CMP	Co^{3+}	--	--	Oxidation	43
TPBCz-CMP	Ag^{+}	--			

Table S3: Table for capacity of POPs-based adsorbents for uranium (UO_2^{2+}) capture.

POPs	pH	U Capacity	References
PAF-1-CH2AO	6.0	300	44
PAF-1-NH(CH2)2AO	6.0	385	45
PAF-170-AO	6.0	702	46
POP-oNH2-AO	--	530	47
COP-CN	4.5	214	48
HCMPs	--	450	49
POP-AOF	7.0	584	50
MA-U-PA	1.0	106.7	51
HTC-MA-TMA	4.5	271.83	52
ND-AO	4.5	212	53

Table S4: Table for capacity of POPs-based adsorbents for iodine (I_2) vapor capture.

POPs	Temp.	I_2 Capacity (wt%)	References
HCP-V0	348 K	324	54
HCP-V1	348 K	426	
HCP-V2	348 K	525	
THPS	348 K	180	55
THSP-C	348 K	340	
PAF-1	298 K	186	56
JUC-Z2	298 K	144	

PAF-24	348 K	276	57
P-DPDA	348 K	408	
TBTT-CMP@1	350 K	442	58
TBTT-CMP@2	350 K	357	
TBTT-CMP@3	350 K	352	
TTPPA	350 K	490	59
TTDAB	350 K	313	
TBIM	350 K	943	60
HBIM	350 K	811	
TDP	350 K	61	
TTPB	350 K	443	61
TS-TAD	350 K	415	62
CPP2	353 K	200	63
CPP-Tp	348 K	346	64
CPP-Pyr	348 K	297	
CMP-LS5	353 K	440	65
SNCMP-1	350 K	570	66
SNCMP-2	350 K	698	
CBP3	353 K	135	67
CBP5	353 K	166	

Table S5: Table for capacity of POPs-based adsorbents for perrhenate (ReO_4^-) capture.

POPs	**Equilibrium times**	**ReO_4^- Capacity (mg/g)**	**References**
TZ-PAF	30 sec	982	68
SCU-CPN-1	30 sec	999	69
SCU-CPN-2	30 sec	1467	70
SCU-CPN-4	1 min	437	71
ImPOP-1	5 min	640	72
ImCOP	<2 min	1164	73
PPS	150 min	596	74
CPN-tpm	20 min	1133	75
VBCOP	--	444	76
IP_{POP}-3		515.5	77
IP_{POP}-4		350.3	
IP_{POP}-5		610	78
PQA-p$N(Me)_2$Py-I	5 min	997	79
PQA-Py-I	--	849	
PQA-pNH_2Py-I	--	642	
Compound-1	60 min	517	80

Table S6: Table of POP-based materials for carbon dioxide (CO_2) gas capture.

POPs	BET surface area (m^2/g)	Temperature (K)	Pressure (bar)	CO_2 uptake (mmol/g)	Q_{st} (kJ/mol)	Reference
PPN-4	6461	298	50	48.19	NM	81
BILP-2	708	273	1	3.38	28.6	82
BILP-4	1135	273	1	5.34	28.7	
BILP-5	599	273	1	2.9	28.8	
BILP-7	1122	273	1	4.38	27.8	
ALP-1	1235	273	1	5.37	29.2	83
ALP-5	801	273	1	4.46	32.5	84
HCP-BDM	847	273	1	2.87	33.5–25.4	85
HCP-BA	742	273	1	1.92	27.4–24.1	
BILP-6-NH_2	1185	273	1	5.57	29.5	86
p-PDM-DVB	841	273	1	1.25	NM	87
Fe-POP-1	875	273	1	4.30	NM	88
P-PCz	1647	273	1	5.57	30.9	89
PAF-60	1094	273	1	2.53	~34.2	90
PAF-61	793	273	1	1.82	~34.2	
PAF-62	701	273	1	1.69	~34.2	
MOPI-I	206[a]	273	1	3.3	39	91
MOPI-II	644[a]	273	1	2.9	32	
MOPI-III	443[a]	273	1	3.0	32	
MOPI-IV	660[a]	273	1	3.8	31	
MOPI-V	921[a]	273	1	2.9	13	
PINK	2090	273	1	4.11	28.9	92
CTF-TPC	1668	273	1	2.17	32	93
CTF-FL	773	273	1	1.67	35	
TPB	2435	273	1	5.9	NM	94
CTF-BI-4	1025	273	1	2.47	31.7-34.3	95
CTF-BI-11	1549	273	1	2.51	31.7-34.3	
NAN-2	56	273	1	1.49	31.52	96
Ni-Por-1	1711	273	1.08	3.13	24	97
TNP1	1090	273	1	178	37.0	98
TNP4	1348	273	1	196	36.5	
FCDTPA-K-700	2065	273	1.13	6.51	< 30.55	99
Network-1	1980	273	1	3.63	23.3	100
BILP-10	787	273	1	4.02	38.2	101
BILP-11	658	273	1	3.09	32.0	
BILP-12	1497	273	1	5.29	27.6	
BILP-13	677	273	1	2.57	26.7	
PRP-1	835	273	1	2.09	25	102
HAT-CTF-450	756	273	1	2.8	NM	103
HAT-CTF-600	899	273	1	3.0	NM	
HAT-CTF-450/600	1090	273	1	3.0	27.1	
PCN-AD	843	273	1	1.49	NM	104
azo-COP-1	635.8	273	1	2.44	29.3	105
azo-COP-2	729.6	273	1	2.55	24.8	
azo-COP-5	127.6	273	1	2.04	27.3	

azo-COP-6	679.1	273	1	2.22	25.8	
azo-COP-8	472.1	273	1	2.02	25.3	
azo-COP-9	509.6	273	1	2.05	25.3	
azo-COP-11	259.2	273	1	2.13	27.4	
H2tapp–A4	719	273	1	7.88	32.9	106
Pd-tapp–A4	618	273	1	10.52	40.0	
Ni-tapp–A4	695	273	1	8.27	37.5	
Mn-tapp–A4	358	273	1	8.36	36.8	
Fe-tapp–A4	360	273	1	8.22	37.6	
Sn-tapp–A4	384	273	1	9.15	37.7	
HCP-91	1028	273	1	1.69	30.7	107
HCP-94	672	273	1	1.48	32	
[a] Calculated based on the BET equation with Ar/87.3 K						

Table S7: Table for representative examples of POPs for cycloaddition of epoxides with CO_2.

POPs	Active site	Substrate	Reaction conditions	Yield (%)	Reference
CTF-1	Basic amine	Epichlorohydrin	6.9 bar, 130 °C, 4 h	77	108
CTF-1-HSA	Basic amine	Epichlorohydrin	6.9 bar, 130 °C, 4 h	96	
CTF-P-HSA	Basic amine	Epichlorohydrin	6.9 bar, 130 °C, 4 h	95	
cCTF	Dicationic viologen, Cl^-	Epichlorohydrin	10 bar, 90 °C, 12 h	95	109
P(DVB-yEVIBr)	Imidazolium and Br^-	Propylene oxide	25 bar, 140 °C, 24 h	92	110
PDMBr	Imidazolium and Br^-	Styrene oxide	10 bar, 110 °C, 4 h	97	111
PAD-3	OH^-, amine	Epichlorohydrin	1 atm, 70 °C, 24 h	97	112
DVB-HTA	AOH, Br^-	Epichlorohydrin	12 bar, 120 °C, 3 h	88	113
POMn-IM	Imidazolium	Epichlorohydrin	10 bar, 120 °C, 8 h	86	114
PCP-Cl	Cl^-	Epichlorohydrin	30 bar, 100 °C, 12 h	98	115
PPh_3-ILBr-ZnX_2@POPs	Zn^{2+}, Br^-	Propylene oxide	30 bar, 120 °C, 1 h	44	116
Al-CPOP	Al^{3+} and Cl^-	Epichlorohydrin	1 atm,120 °C, 24 h	94	117
DVB@ISA	Al^{3+} and Br^-	Epichlorohydrin	10 bar, 60 °C, 24 h	99	118
Co/POP-TPP	Co^{3+}	Epichlorohydrin	1 atm, 29 °C, 24 h	95	119

Al-HCP	Al^{3+}	Propylene oxide	10 bar, 40 °C, 1 h	99	120
Co-CMP	Co^{3+}	Propylene oxide	1 atm, 25 °C, 48 h	82	121
Co-MON	Co^{3+}	Propylene oxide	10 bar, 60 °C, 12 h	75	122
Bp-Zn@MA	Zn^{2+}	Propylene oxide	10 bar, 100 °C, 1.5 h	99	123
PRP-1	AOH	Epichlorohydrin	1 bar, 60 °C, 24 h	89	124
NP-NHC	NHC	Propylene oxide	1 bar, 120 °C, 24 h	98	125

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