Computational evaluation of aluminophosphate zeotypes for CO_2/N_2 separation

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SUPPORTING INFORMATION

Table S1: List of AlPO topologies used, name of material with aluminophosphate-based (or related) composition, space group, lattice parameters obtained from PBE-TS calculations, and size of k-mesh used in the calculations. The cell parameters given refer to the conventional cell setting. Systems that were optimised in a smaller, primitive cell are marked by an asterisk; in these cases, the k-mesh refers to the primitive cell.

a) Frameworks that have been reported as AlPOs

FTC	Material	Space group	a / Å	b / Å	c / Å	α / deg	β / deg	γ / deg	k-mesh
AEI*	AlPO-18[1]	$C2/c$	13.802	12.787	18.649	90	89.817	90	1×1×1
AEL	AlPO-11[2]	$Ibm2$	13.552	18.912	8.403	90	90	90	2×2×2
AEN	AlPO-53B[3]	$Pbca$	18.132	13.945	9.698	90	90	90	1×1×1
AET*	AlPO-8[4]	$Cmc2_1$	33.746	14.485	8.333	90	90	90	1×1×2
AFI	AlPO-5[5]	$P6cc$	13.972	13.972	8.645	90	90	120	2×2×2
AFN	AlPO-14[6]	$P\bar{1}$	9.713	9.748	10.145	78.214	78.089	87.829	2×2×2
AFO	AlPO-41[7]	$P2_1$	9.745	13.933	8.295	90	90	112.167	2×2×2
AFR	AlPO-40[8]	$Pccn$	22.389	13.832	14.118	90	90	90	2×2×2
AFT	AlPO-52[9]	$P\bar{3}1c$	13.806	13.806	29.902	90	90	120	1×1×2
APC	$AlPO_4$-C[10]	$Pbca$	20.228	9.688	8.727	90	90	90	2×2×2
ATO	AlPO-31[11]	$R\bar{3}$	20.838	20.838	5.002	90	90	120	1×1×3
ATS	AlPO-36[12]	$P\bar{1}$	13.135	21.599	5.120	89.785	94.343	89.968	2×1×4
ATT	AlPO-33[13]	$P2_12_12_1$	9.896	15.202	9.568	90	90	90	2×2×2
ATV	AlPO-25[14]	$Abm2$	9.791	15.302	8.640	90	90	90	2×2×2
AWW	AlPO-22[15]	$P4/ncc$	13.807	13.807	15.466	90	90	90	2×2×2
CHA	AlPO-34[16]	$R\bar{3}$	13.792	13.792	14.972	90	90	120	1×1×1
ERI	AlPO-17[17]	$P6_3/m$	13.205	13.205	15.385	90	90	120	1×1×1
EZT	EMM-3[18]	$I2/m$	10.301	12.706	22.015	89.652	90	90	2×2×1
FAU*	AlPO-37[19]	$Fd\bar{3}$	24.685	24.685	24.685	90	90	90	1×1×1
GIS	AlPO-43[20]	$Fddd$	13.979	13.778	10.349	90	90	90	1×1×1
LEV*	AlPO-35[21]	$R\bar{3}c$	13.271	13.271	45.889	90	90	120	2×2×2
LTA*	AlPO-42[22]	$Fm\bar{3}c$	24.100	24.100	24.100	90	90	90	2×2×2
OSI	UiO-6[23]	$Imm2$	18.462	18.429	5.045	90	90	90	2×2×4
PON	IST-1[24]	$Pca2_1$	8.974	9.334	16.120	90	90	90	4×4×2
SAF	STA-15[25]	$Iba2$	14.870	27.857	8.414	90	90	90	2×2×2
SAS	AlPO-SAS[26]	$P2_1/n$	10.108	14.685	13.701	90	88.139	90	2×1×1
SAT*	STA-2[27]	$R\bar{3}$	13.002	13.002	30.796	90	90	120	2×2×2
SFO*	SSZ-51[28]	$C2/c$	22.682	13.811	14.122	90	98.795	90	2×2×2
VFI	VPI-5[29]	$P6_3cm$	18.806	18.806	8.624	90	90	120	1×1×2

ZON	UiO-7[30]	$Pbca$	14.053	15.184	17.480	90	90	90	2×2×2

b) Frameworks that have been reported as SAPOs or MeAPOs

FTC	Material	Space group	a / Å	b / Å	c / Å	α / deg	β / deg	γ / deg	k-mesh
ACO	ACP-1[31]	$I\bar{4}2m$	10.008	10.008	10.009	90	90	90	2×2×2
AFS	MAPSO-46[32]	$P3c1$	13.245	13.245	26.316	90	90	120	2×2×1
AFV	ZnAPO-57[33]	$P\bar{3}c1$	13.389	13.389	25.549	90	90	120	2×2×1
AFX	SAPO-56[34]	$P\bar{3}1c$	13.774	13.774	20.048	90	90	120	1×1×1
AFY	MnAPO-50[35]	$P\bar{3}$	12.530	12.530	8.740	90	90	120	2×2×2
ATN	MAPO-39[36]	$I4/m$	13.175	13.175	5.311	90	90	90	2×2×4
AVL	ZnAPO-59[33]	$P\bar{3}c1$	13.496	13.496	35.587	90	90	120	1×1×2
BPH	STA-5[37]	$P321$	13.247	13.247	13.152	90	90	120	2×2×2
DFT	ACP-3[38]	$P4_2/n$	10.168	10.168	8.356	90	90	90	2×2×2
GME	STA-19[39]	$P\bar{3}1c$	13.836	13.836	9.917	90	90	120	2×2×2
IFO	ITQ-51[40]	$P2_1/n$	23.273	16.583	4.977	90	90.615	90	1×1×4
JRY	CoAPO-CJ40[41]	$P2_12_12_1$	8.223	9.235	17.575	90	90	90	2×2×2
JSN	CoAPO-CJ69[42]	$P2_1/c$	8.816	14.040	15.157	90	96.695	90	2×1×1
KFI	STA-14[43]	$Pn\bar{3}n$	18.780	18.780	18.780	90	90	90	2×2×2
MER*	ACP-MER[31]	$Ccca$	19.681	20.137	9.954	90	90	90	2×2×2
OWE	UiO-28[44]	$Pbcm$	9.218	14.342	14.530	90	90	90	2×2×2
PHI	ACP-PHI[31]	$C2/c$	9.917	14.267	14.187	90	90.333	90	2×2×2
RHO*	DNL-6[45]	$I23$	15.123	15.123	15.123	90	90	90	1×1×1
SAO	STA-1[46]	$P\bar{4}n2$	13.811	13.811	21.871	90	90	90	2×2×2
SAV	STA-7[47]	$P4/n$	18.666	18.666	9.453	90	90	90	2×2×2
SIV*	SIZ-7[48]	$C2/c$	9.831	14.297	28.502	90	90.390	90	2×2×1

Table S2: Results of preliminary simulations for 51 AlPO frameworks: Henry constants K_H of CO_2 and N_2, ratio of the Henry constants, CO_2 uptakes at three different pressures (15, 75, 150 kPa), and difference in CO_2 uptake ("Delta loading") between 75/150 kPa and 15 kPa. The framework type codes of those systems for which further calculations were performed are highlighted.

FTC	$K_H(CO_2)$	K_H(N2)	$K_H(CO_2)$ / $K_H(N_2)$	$n(CO_2)$	$n(CO_2)$	$n(CO_2)$	$\Delta n(CO_2)$	$\Delta n(CO_2)$
				15 kPa	75 kPa	150 kPa	75 kPa - 15 kPa	150 kPa - 15kPa
	mmol (g·bar)$^{-1}$	mmol (g·bar)$^{-1}$		mmol g^{-1}	mmol g^{-1}	mmol g^{-1}	mmol g^{-1}	mmol g^{-1}
ACO	2.312	0.087	26.6	0.319	1.216	1.858	0.897	1.539
AEI	2.304	0.161	14.3	0.346	1.625	2.685	1.279	2.339
AEL	2.039	0.125	16.3	0.264	0.820	1.092	0.556	0.828
AEN	2.505	0.032	79.5	0.341	1.131	1.552	0.790	1.211
AET	0.386	0.051	7.6	0.059	0.321	0.675	0.261	0.615
AFI	0.571	0.080	7.1	0.086	0.442	0.860	0.356	0.774
AFN	2.923	0.085	34.3	0.388	1.334	1.904	0.946	1.516
AFO	2.391	0.132	18.1	0.302	0.870	1.126	0.568	0.824
AFR	1.266	0.116	10.9	0.194	1.007	1.961	0.813	1.767
AFS	1.345	0.114	11.8	0.200	1.018	2.013	0.818	1.813
AFT	4.077	0.184	22.1	0.482	1.740	2.773	1.258	2.291
AFV	3.332	0.231	14.4	0.458	1.689	2.502	1.230	2.043
AFX	5.061	0.192	26.3	0.549	1.771	2.767	1.222	2.218
AFY	2.884	0.146	19.8	0.425	2.056	3.635	1.631	3.209
APC	2.569	0.029	88.7	0.342	1.167	2.019	0.824	1.677
ATN	20.254	0.274	74.0	1.322	1.938	2.129	0.616	0.807
ATO	1.567	0.125	12.5	0.206	0.685	0.943	0.478	0.737
ATS	1.401	0.115	12.2	0.217	1.074	1.797	0.857	1.580
ATT	12.784	0.184	69.7	1.306	2.442	2.775	1.136	1.468
ATV	2.810	0.149	18.9	0.322	0.853	1.138	0.531	0.816
AVL	4.729	0.234	20.2	0.561	1.831	2.658	1.270	2.097
AWW	3.162	0.214	14.8	0.440	1.589	2.267	1.149	1.827
BPH	1.653	0.121	13.7	0.234	1.169	2.275	0.935	2.041
CHA	2.634	0.188	14.0	0.392	1.713	2.812	1.321	2.420
DFT	1.805	0.067	26.9	0.238	0.794	1.145	0.556	0.906
ERI	2.254	0.184	12.2	0.321	1.285	1.955	0.964	1.634
EZT	1.614	0.152	10.6	0.233	0.970	1.522	0.737	1.290
FAU	0.407	0.080	5.1	0.062	0.329	0.713	0.267	0.651
GIS	13.482	0.138	97.9	1.990	3.627	3.875	1.636	1.884
GME	7.070	0.166	42.5	0.642	1.727	2.598	1.085	1.956
IFO	0.385	0.059	6.5	0.058	0.308	0.642	0.249	0.583
JRY	6.647	0.181	36.7	0.751	1.814	2.218	1.063	1.467
JSN	4.079	0.222	18.4	0.503	1.418	1.819	0.915	1.317
KFI	3.870	0.164	23.6	0.529	2.070	3.245	1.541	2.716
LEV	3.615	0.243	14.9	0.483	1.668	2.479	1.185	1.996
LTA	0.947	0.114	8.3	0.144	0.776	1.694	0.632	1.550

MER	3.155	0.109	28.9	0.419	1.452	2.180	1.033	1.761
OSI	0.745	0.083	9.0	0.108	0.445	0.706	0.338	0.598
OWE	5.788	0.229	25.3	0.720	2.008	2.630	1.287	1.910
PHI	6.202	0.151	40.9	0.741	2.030	2.702	1.290	1.962
PON	3.809	0.132	28.8	0.497	1.528	2.016	1.032	1.519
RHO	2.470	0.178	13.9	0.356	1.574	2.712	1.217	2.356
SAF	0.586	0.070	8.4	0.088	0.430	0.760	0.341	0.672
SAO	0.741	0.119	6.2	0.113	0.589	1.239	0.477	1.126
SAS	1.903	0.180	10.6	0.277	1.200	1.943	0.923	1.666
SAT	1.979	0.176	11.3	0.278	1.049	1.572	0.772	1.294
SAV	2.973	0.174	17.0	0.420	1.796	3.053	1.376	2.632
SFO	1.237	0.113	10.9	0.190	0.983	1.922	0.793	1.732
SIV	9.560	0.147	64.9	1.259	2.789	3.270	1.530	2.011
VFI	0.218	0.050	4.3	0.033	0.169	0.352	0.137	0.319
ZON	4.793	0.231	20.7	0.565	1.451	1.839	0.886	1.273

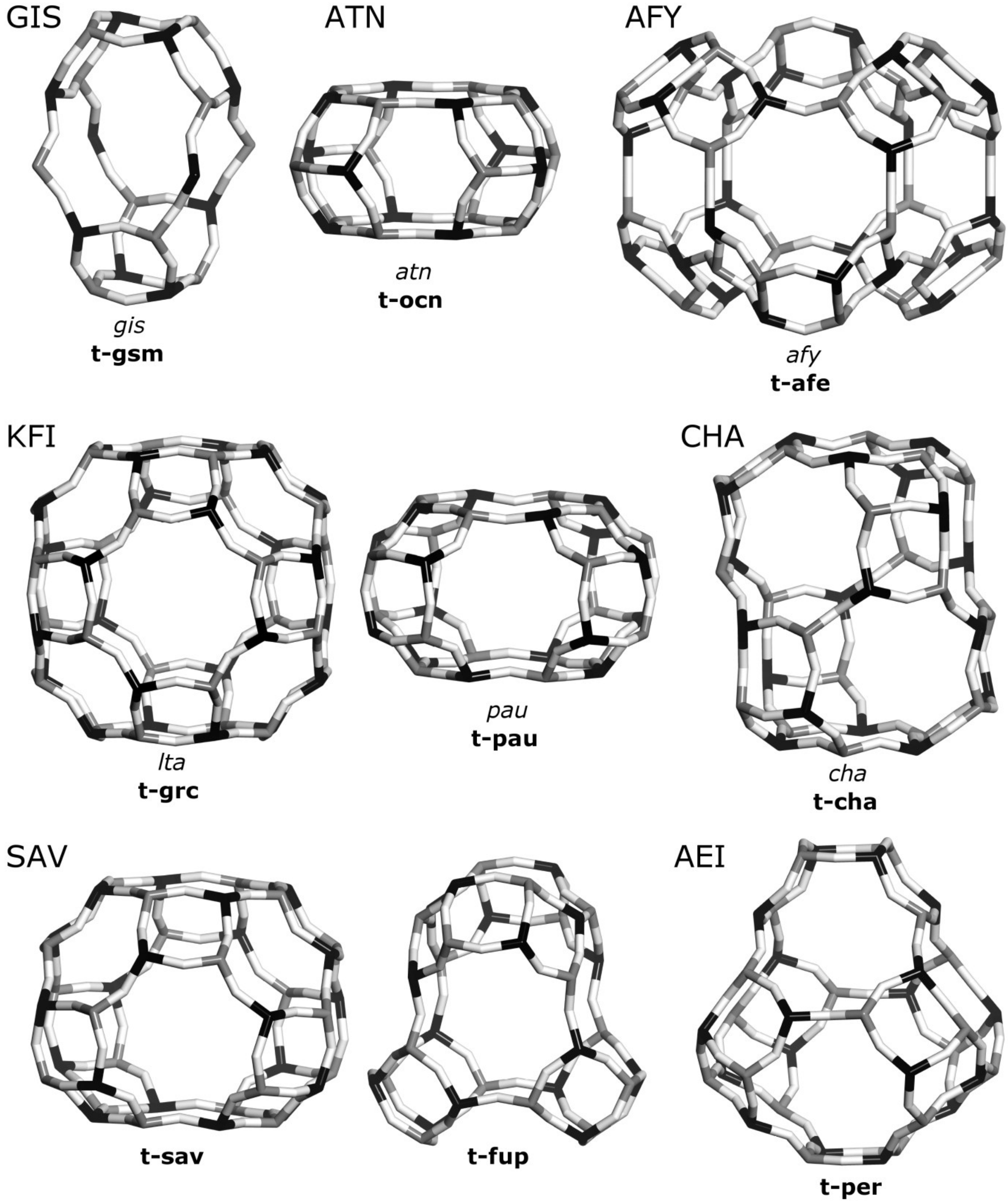

Figure S1: Visualisation of cages occurring in those AlPOs for which interaction energy maps were computed. The cages are labelled according to the composite building unit (where available) and natural tiling nomenclatures, with labels given in italic and bold letters, respectively.[49,50]

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