Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Zeolite Screening for the Separation of Mixtures Containing SO_2, CO_2 and CO gases

Electronic Supporting Information

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Table S1. Topological and geometrical parameters describing pore systems in IZA zeolites. Each structure is characterized in terms of number of pore systems (#PS). For structures with #PS>0, each pore system (PS ID) is characterized in terms of dimensionality (dim), the diameter of the largest spheres: included (Di), free (Df) and included along free sphere path (Dif) as well as the character of the pore system (C- channel, IC – interconnected cage).

Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC	Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC
ABW	2	0	3.61	3.1	3.61	1	C	APD	4	0	4.19	3.23	4.19	1	C
		1	3.61	3.1	3.61	1	C			1	4.2	3.23	4.2	1	C
ACO	1	0	3.9	3.16	3.9	3	C			2	4.2	3.23	4.2	1	C
AEI	1	0	6.9	3.44	6.9	3	IC			3	4.19	3.23	4.19	1	C
AEL	2	0	5.22	4.07	5.22	1	C	AST	0						
		1	5.22	4.07	5.22	1	C	ASV	1	0	4.95	4.03	4.95	1	C
AEN	2	0	3.9	3.18	3.9	2	C	ATN	2	0	5.51	3.71	5.51	1	C
		1	3.9	3.18	3.9	2	C			1	5.51	3.71	5.51	1	C
AET	2	0	7.77	7.16	7.77	1	C	ATO	3	0	5.34	5.09	5.34	1	C
		1	7.77	7.16	7.77	1	C			1	5.34	5.09	5.34	1	C
AFG	0									2	5.34	5.09	5.34	1	C
AFI	1	0	7.56	7.02	7.56	1	C	ATS	2	0	6.57	6.36	6.57	1	C
AFN	2	0	4.75	3.09	4.75	1	IC			1	6.57	6.36	6.57	1	C
		1	4.75	3.09	4.75	1	IC	ATT	1	0	4.88	3.39	4.88	2	C
AFO	2	0	5.03	4.33	5.03	1	C	ATV	2	0	3.9	3.04	3.9	1	C
		1	5.03	4.33	5.03	1	C			1	3.9	3.04	3.9	1	C
AFR	2	0	7.82	6.57	7.82	2	C	AWO	4	0	4.49	3.26	4.49	1	C
		1	7.82	6.57	7.82	2	C			1	4.49	3.26	4.49	1	C
AFS	1	0	9.11	5.61	9.11	3	IC			2	4.48	3.26	4.48	1	C
AFT	1	0	7.14	3.28	7.14	3	IC			3	4.48	3.26	4.48	1	C
AFX	1	0	7.11	3.33	7.11	3	IC	AWW	2	0	6.9	3.77	6.9	1	IC
AFY	1	0	7.42	5.5	7.42	3	C			1	6.88	3.77	6.88	1	IC
AHT	0							BCT	0						
ANA	0							BEA	1	0	6.1	5.63	6.1	3	C
APC	0							BEC	1	0	6.23	5.91	6.23	3	C

Table S2. Topological and geometrical parameters describing pore systems in IZA zeolites. Each structure is characterized in terms of number of pore systems (#PS). For structures with #PS>0, each pore system (PS ID) is characterized in terms of dimensionality (dim), the diameter of the largest spheres: included (Di), free (Df) and included along free sphere path (Dif) as well as character the of the pore system (C- channel, IC – interconnected cage).

Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC	Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC
BIK	2	0	3.76	3.14	3.76	1	C	CON	1	0	6.77	5.2	6.77	3	C
		1	3.76	3.14	3.76	1	C	CZP	1	0	3.75	3.24	3.75	1	C
BOF	2	0	5.15	4.18	5.15	1	C	DAC	2	0	4.79	3.4	4.79	2	C
		1	5.15	4.17	5.15	1	C			1	4.79	3.4	4.79	2	C
BOG	1	0	7.49	6.48	7.49	3	C	DDR	3	0	7.06	3.25	7.06	2	IC
BPH	1	0	9.11	5.61	9.11	3	IC			1	7.06	3.25	7.06	2	IC
BRE	0									2	7.06	3.25	7.06	2	IC
BSV	2	0	4.76	3.44	4.76	3	C	DFO	1	0	10.89	6.79	10.89	3	IC
		1	4.76	3.44	4.76	3	C	DFT	1	0	4.18	3.25	4.18	1	C
CAN	1	0	5.76	5.42	5.76	1	C	DOH	0						
CAS	0							DON	2	0	8.17	7.67	8.17	1	C
CDO	2	0	4.97	3.04	4.97	2	IC			1	8.17	7.67	8.17	1	C
		1	4.97	3.04	4.97	2	IC	EAB	2	0	6.62	3.14	6.62	2	IC
CFI	2	0	7.07	6.86	7.07	1	C			1	6.61	3.14	6.61	2	IC
		1	7.07	6.86	7.07	1	C	EDI	1	0	4.86	3.04	4.86	1	IC
CGF	0							EMT	1	0	10.99	6.97	10.99	3	IC
CGS	2	0	5.3	3.61	5.3	1	C	EON	3	0	5.6	2.84	5.6	2	IC
		1	5.31	3.61	5.31	1	C			1	7.27	6.39	7.27	1	C
CHA	1	0	6.74	3.32	6.74	3	IC			2	7.27	6.39	7.27	1	C
CHI	4	0	3.51	3.23	3.51	1	C	EPI	2	0	4.92	3.22	4.92	2	IC
		1	3.51	3.23	3.51	1	C			1	4.92	3.22	4.92	2	IC
		2	3.51	3.23	3.51	1	C	ERI	1	0	6.3	3.02	6.3	3	IC
		3	3.51	3.23	3.51	1	C	ESV	2	0	5.67	3.25	5.67	1	IC
CLO	2	0	15.32	5.91	15.32	3	IC			1	5.67	3.26	5.67	1	IC
		1	10.18	3.79	10.18	3	IC	ETR	1	0	9.61	8.92	9.61	1	C

Table S3. Topological and geometrical parameters describing pore systems in IZA zeolites. Each structure is characterized in terms of number of pore systems (#PS). For structures with #PS>0, each pore system (PS ID) is characterized in terms of dimensionality (dim), the diameter of the largest spheres: included (Di), free (Df) and included along free sphere path (Dif) as well as the character of the pore system (C- channel, IC – interconnected cage).

Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC	Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC
EUO	2	0	6.26	4.54	6.26	1	C	ISV	1	0	6.36	5.78	6.36	3	C
		1	6.26	4.54	6.26	1	C	ITE	4	0	7.77	3.81	7.77	1	IC
EZT	2	0	5.9	5.61	5.9	1	C			1	7.77	3.81	7.77	1	IC
		1	5.91	5.61	5.91	1	C			2	7.77	3.81	7.77	1	IC
FAR	0									3	7.77	3.81	7.77	1	IC
FAU	1	0	10.7	6.95	10.7	3	IC	ITH	1	0	6.28	4.67	6.28	3	C
FER	2	0	5.41	4.29	5.16	2	C	ITR	1	0	5.96	4.71	5.96	3	C
		1	5.41	4.29	5.16	2	C	ITW	2	0	4.16	3.47	4.16	1	C
FRA	0									1	4.16	3.47	4.16	1	C
GIS	1	0	4.57	2.87	4.57	3	IC	IWR	1	0	6.9	5.51	6.9	3	C
GIU	0						C	IWS	1	0	7.62	6.26	7.62	3	C
GME	1	0	7.11	6.68	7.11	3	C	IWV	2	0	8.12	6.63	8.12	2	C
GON	2	0	5.66	4.87	5.66	1	C			1	8.12	6.63	8.12	2	C
		1	5.66	4.87	5.66	1	C	IWW	1	0	6.55	5.84	6.55	3	C
GOO	0							JBW	1	0	3.85	3.32	3.85	1	C
HEU	4	0	5.21	3.27	5.21	1	IC	JRY	2	0	4.1	3.72	4.1	1	C
		1	4.68	3.1	4.68	1	IC			1	4.1	3.72	4.1	1	C
		2	4.68	3.1	4.68	1	IC	KFI	1	0	10.17	3.64	10.17	3	IC
		3	5.21	3.27	5.21	1	IC	LAU	2	0	5.47	3.67	5.47	1	C
IFR	2	0	6.56	5.98	6.56	1	C			1	5.47	3.67	5.47	1	C
		1	6.56	5.98	6.56	1	C	LEV	3	0	6.39	3.13	6.39	2	IC
IHW	2	0	6.07	3.27	6.07	2	IC			1	6.39	3.13	6.39	2	IC
		1	6.07	3.27	6.07	2	IC			2	6.39	3.13	6.39	2	IC
IMF	2	0	6.68	4.87	6.68	2	C	LIO	0						
		1	6.68	4.87	6.68	2	C	LIT	0						

Table S4. Topological and geometrical parameters describing pore systems in IZA zeolites. Each structure is characterized in terms of number of pore systems (#PS). For structures with #PS>0, each pore system (PS ID) is characterized in terms of dimensionality (dim), the diameter of the largest spheres: included (Di), free (Df) and included along free sphere path (Dif) as well as the character of the pore system (C- channel, IC – interconnected cage).

Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC	Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC
LOS	0							MRE	2	0	5.73	5.19	5.73	1	C
LOV	1	0	4.25	3.38	3.73	3	C			1	5.73	5.18	5.73	1	C
LTA	1	0	10.24	3.81	10.24	3	IC	MSE	1	0	6.49	5.98	6.49	3	C
LTF	2	0	7.76	7.1	7.76	1	C	MSO	0						
		1	6.51	6	6.51	3	C	MTF	2	0	5.58	3.63	5.58	1	IC
LTL	1	0	9.61	7.1	9.61	1	C			1	5.58	3.63	5.58	1	IC
LTN	0							MTN	0						
MAR	0							MTT	2	0	5.52	4.55	5.52	1	C
MAZ	2	0	7.69	7.1	7.69	1	C			1	5.52	4.54	5.52	1	C
		1	5.63	2.85	5.63	3	IC	MTW	2	0	5.31	5.08	5.31	1	C
MEI	1	0	7.66	6.45	7.66	1	C			1	5.31	5.08	5.31	1	C
MEL	1	0	6.87	4.77	6.87	3	C	MVY	0						
MEP	0							MWW	2	0	9.29	3.98	9.29	2	IC
MER	4	0	6.25	3.8	6.25	1	IC			1	5.73	4.17	5.73	2	C
		1	3.59	2.8	3.59	1	C	NAB	1	0	3.76	3.09	3.76	3	C
		2	6.25	3.8	6.25	1	IC	NAT	4	0	3.95	3.84	3.95	1	C
		3	3.59	2.8	3.59	1	C			1	3.95	3.84	3.95	1	C
MFI	1	0	5.94	4.28	5.94	3	C			2	3.95	3.84	3.95	1	C
MFS	2	0	6.21	4.94	6.21	1	C			3	3.95	3.84	3.95	1	C
		1	6.21	4.94	6.21	1	C	NES	2	0	6.17	4.66	6.17	2	C
MON	1	0	3.74	3.13	3.74	3	C			1	6.17	4.66	6.17	2	C
MOR	2	0	6.2	6.03	6.2	1	C	NON	0						
		1	6.2	6.03	6.2	1	C	NPO	1	0	3.34	3.1	3.34	1	C
MOZ	2	0	9.63	7.14	9.63	1	C	NSI	2	0	3.45	2.87	3.45	1	C
		1	6.5	6.05	6.48	3	C			1	3.45	2.87	3.45	1	C

Table S5. Topological and geometrical parameters describing pore systems in IZA zeolites. Each structure is characterized in terms of number of pore systems (#PS). For structures with #PS>0, each pore system (PS ID) is characterized in terms of dimensionality (dim), the diameter of the largest spheres: included (Di), free (Df) and included along free sphere path (Dif) as well as the character of the pore system (C- channel, IC – interconnected cage).

Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC	Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC
OBW	1	0	8.86	4.78	8.86	3	IC	RWR	4	0	3.92	2.83	3.92	1	C
OFF	1	0	6.49	6.04	6.49	3	C			1	3.92	2.83	3.92	1	C
OSI	2	0	6.26	5.88	6.26	1	C			2	3.92	2.83	3.92	1	C
		1	6.26	5.88	6.26	1	C			3	3.92	2.83	3.92	1	C
OSO	1	0	5.67	5.47	5.67	3	C	RWY	1	0	14	5.89	14	3	IC
OWE	1	0	5.2	3.38	5.2	2	IC	SAF	2	0	6.23	5.73	6.23	1	C
PAR	2	0	3.68	3.19	3.68	1	C			1	6.23	5.73	6.23	1	C
		1	3.68	3.19	3.68	1	C	SAO	1	0	8.22	6.28	8.22	3	C
PAU	3	0	10.08	3.66	10.08	3	IC	SAS	2	0	8.53	3.82	8.53	1	IC
		1	6.22	3.3	6.22	3	IC			1	8.54	3.82	8.54	1	IC
		2	10.08	3.66	10.08	3	IC	SAT	1	0	6.17	2.85	6.17	3	IC
PHI	2	0	5	3.23	5	2	IC	SAV	1	0	8.28	3.7	8.28	3	IC
		1	5	3.23	5	2	IC	SBE	2	0	12.09	6.81	12.09	3	IC
PON	2	0	4.5	3.9	4.5	1	C			1	12.09	6.81	12.09	3	IC
		1	4.5	3.9	4.5	1	C	SBN	2	0	4.39	3.4	4.39	2	C
PUN	1	0	4.98	3.95	4.97	3	C			1	4.4	3.4	4.4	2	C
RHO	2	0	10.03	3.66	10.03	3	IC	SBS	1	0	10.97	6.87	10.97	3	IC
		1	10.03	3.66	10.03	3	IC	SBT	1	0	10.39	6.94	10.38	3	C
RRO	2	0	3.87	3.51	3.87	1	C	SFE	1	0	6.23	5.81	6.23	1	C
		1	3.87	3.51	3.87	1	C	SFF	2	0	7.07	4.94	7.07	1	C
RSN	2	0	4.24	3.37	3.73	2	C			1	7.08	4.94	7.08	1	C
		1	4.24	3.37	3.73	2	C	SFG	1	0	6.35	4.98	6.35	2	C
RTE	2	0	6.4	3.58	6.4	1	IC	SFH	4	0	7.66	6.36	7.66	1	C
		1	6.4	3.58	6.4	1	IC			1	7.66	6.36	7.66	1	C
RTH	2	0	7.63	3.74	7.63	1	IC			2	7.66	6.35	7.66	1	C
		1	7.63	3.74	7.63	1	IC			3	7.66	6.35	7.66	1	C
RUT	0							SFN	2	0	7.46	6.3	7.46	1	C
										1	7.46	6.3	7.46	1	C

Table S6. Topological and geometrical parameters describing pore systems in IZA zeolites. Each structure is characterized in terms of number of pore systems (#PS). For structures with #PS>0, each pore system (PS ID) is characterized in terms of dimensionality (dim), the diameter of the largest spheres: included (Di), free (Df) and included along free sphere path (Dif) as well as the character of the pore system (C- channel, IC – interconnected cage).

Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC	Zeolite	#PS	PS ID	Di	Df	Dif	dim	PC
SFO	2	0	7.48	6.55	7.48	2	C	TOL	0						
		1	7.48	6.55	7.48	2	C	TON	2	0	5.04	4.65	5.04	1	C
SFS	1	0	7.03	5.47	7.03	2	C			1	5.04	4.65	5.04	1	C
SGT	0							TSC	1	0	15.86	3.68	15.85	3	IC
SIV	1	0	4.98	3.28	4.98	3	IC	TUN	1	0	8.04	4.99	8.04	3	IC
SOD	0							UEI	4	0	5.11	3.36	5.11	1	IC
SOF	1	0	4.74	3.82	4.74	3	C			1	5.11	3.36	5.11	1	IC
SOS	2	0	4.38	3.81	4.38	1	C			2	5.11	3.36	5.11	1	IC
		1	4.38	3.82	4.38	1	C			3	5.11	3.36	5.11	1	IC
SSF	1	0	7.26	5.76	7.26	2	C	UFI	2	0	9.69	3.49	9.69	2	IC
SSY	2	0	6.92	5.54	6.92	1	C			1	9.69	3.49	9.69	2	IC
		1	6.93	5.53	6.93	1	C	UOS	2	0	5.3	3.73	5.3	1	C
STF	2	0	7.22	5.04	7.22	1	C			1	5.3	3.74	5.3	1	C
		1	7.22	5.04	7.22	1	C	UOZ	0						
STI	4	0	5.81	4.53	5.81	1	C	USI	2	0	6.32	5.84	6.32	2	C
		1	5.81	4.54	5.81	1	C			1	6.32	5.84	6.32	2	C
		2	5.81	4.54	5.81	1	C	UTL	2	0	8.7	7.12	8.7	2	C
		3	5.81	4.54	5.81	1	C			1	8.7	7.12	8.7	2	C
STO	4	0	6.4	5.35	6.4	1	C	VET	1	0	5.99	5.58	5.99	1	C
		1	5.75	4.96	5.75	1	C	VFI	1	0	11.4	10.99	11.4	1	C
		2	6.31	5.61	6.31	1	C	VNI	0						
		3	6.35	5.39	6.35	1	C	VSV	4	0	3.73	3.37	3.73	2	C
STT	2	0	6.56	3.66	6.56	1	IC			1	3.73	3.37	3.73	2	C
		1	6.56	3.66	6.56	1	IC			2	3.73	3.37	3.73	2	C
STW	1	0	4.9	4.48	4.9	3	C			3	3.73	3.37	3.72	2	C
SVR	1	0	5.34	4.55	5.34	3	C	WEI	1	0	3.79	3.03	3.79	3	C
SZR	1	0	5.58	4.29	5.58	3	C	WEN	1	0	4.96	3.62	4.96	2	C
TER	2	0	6.17	4.68	6.17	2	C	YUG	0						
		1	6.17	4.68	6.16	2	C	ZON	2	0	5.2	3.12	5.2	1	IC
THO	2	0	4.47	3.29	4.47	1	C			1	5.2	3.12	5.2	1	IC
		1	4.48	3.29	4.48	1	C								

Table S7. Unit cell length and angle, pore volume, surface area, and references of the crystallographic positions *of some representative zeolites used in this study. The selection is based on pore character and pore space dimensionality.*

Zeolite	Crystallographic positions	Unit cell			Angles unit cell			Pore Volume	SSA (Helium)
		a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	(cm^3/g)	(m^2/g)
ASV	Baerlocher et al.	8.67	8.67	13.92	90	90	90	0.10	305.30
DON	Wessels et al.	14.97	8.48	30.03	90	102.65	90	0.17	508.77
ITW	Baerlocher et al.	10.45	15.03	8.95	90	90	90	0.10	382.27
JRY	Baerlocher et al.	8.17	9.20	17.29	90	90	90	0.09	333.56
LAU	Artioli and Stahl	14.85	13.17	7.54	90	110.32	90	0.13	471.29
LTL	Newsam	18.47	18.47	7.48	90	90	120	0.17	553.03
MOR	Gramlich	18.11	20.53	7.53	90	90	90	0.15	477.93
NAT	Baerlocher et al.	13.85	13.85	6.42	90	90	90	0.12	436.30
PON	Baerlocher et al.	8.91	9.21	16.09	90	90	90	0.09	329.22
AFR	Baerlocher et al.	22.31	13.57	6.97	90	90	90	0.25	817.97
FER	Morris et al.	18.72	14.07	7.42	90	90	90	0.13	407.45
IWV	Baerlocher et al.	27.83	26.08	13.94	90	90	90	0.27	883.36
NES	Baerlocher et al.	26.06	13.88	22.86	90	90	90	0.19	701.99
SFO	Baerlocher et al.	22.59	12.57	6.97	90	99.02	90	0.25	815.75
SFG	Baerlocher et al.	25.53	12.58	13.07	90	90	90	0.14	494.75
TER	Baerlocher et al.	9.81	23.65	20.24	90	90	90	0.18	647.26
AFY	Baerlocher et al.	12.33	12.33	8.60	90	90	120	0.29	1208.05
BEC	Baerlocher et al.	12.77	12.77	12.98	90	90	90	0.28	979.93
BOG	Pluth and Smith	20.24	23.80	12.80	90	90	90	0.24	817.50
MEL	Fyfe et al.	20.07	20.07	13.41	90	90	90	0.15	544.96
MFI	van Koningsveld et al.	20.02	19.90	13.38	90	90	90	0.16	547.66
ITR	Baerlocher et al.	11.67	21.97	25.17	90	90	90	0.16	572.09
SBT	Baerlocher et al.	17.19	17.19	41.03	90	90	120	0.34	1057.79
STW	Baerlocher et al.	11.89	11.89	29.92	90	90	120	0.20	804.89
SZR	Baerlocher et al.	18.87	14.40	7.51	90	90	90	0.12	398.51
ITQ-3	Camblor et al.	20.62	9.72	19.62	90	90	90	0.23	693.71
MTF	Baerlocher et al.	9.63	30.39	7.25	90	90.45	90	0.09	263.69
SAS	Baerlocher et al.	14.35	14.35	10.40	90	90	90	0.26	794.61
DDR	Gies	13.86	13.86	40.89	90	90	120	0.14	400.48
LEV	Merlino and Alberti	13.34	13.34	23.01	90	90	120	0.15	706.26
MWW	Baerlocher et al.	14.39	14.39	25.20	90	90	120	0.23	801.23
CHA	Calligaris et al.	9.46	9.46	9.46	94.1	94.1	94.1	0.25	893.81
ERI	Gard et al.	13.27	13.27	15.05	90	90	120	0.22	716.96
FAU	Hriljac et al.	24.26	24.26	24.26	90	90	90	0.33	1020.96
ITQ-29	Corma et al.	11.87	11.87	11.87	90	90	90	0.29	849.36
KFI	Parise et al.	18.67	18.67	18.67	90	90	90	0.23	786.75
PAU	Gordon et al.	35.09	35.09	35.09	90	90	90	0.16	538.21
RHO	McCusker and Baerlocher	15.03	15.03	15.03	90	90	90	0.25	783.40
SBE	Baerlocher et al.	18.53	18.53	27.13	90	90	90	0.32	938.11

Table S8. Computed amount of adsorbed molecules and adsorption selectivity from the ternary mixture ($SO_2/CO_2/CO$ with ratio 20:40:40). These values were taken from the adsorption isotherms obtained from Monte Carlo simulations at room conditions for temperature and pressure.

Zeolite	SO_2 loading (mol/kg)	CO_2 loading (mol/kg)	CO loading (mol/kg)	S SO_2/CO_2	S CO_2/CO
ASV	1.750	0.040	0.005	86.761	8.730
DON	1.062	0.235	0.016	9.029	14.816
ITW	2.810	0.024	0.008	238.558	3.018
JRY	2.682	0.021	0.002	256.479	9.693
LAU	2.226	0.107	0.003	41.689	31.387
LTL	1.412	0.245	0.014	11.547	17.406
MOR	2.472	0.164	0.004	30.059	40.659
NAT	3.829	0.052	0.007	147.817	7.755
PON	2.620	0.021	0.002	247.229	8.635
AFR	3.055	0.341	0.016	17.928	21.103
FER	2.295	0.021	0.001	220.820	20.079
IWV	3.033	0.362	0.016	16.744	22.008
NES	1.791	0.331	0.010	10.822	33.355
SFO	2.830	0.359	0.017	15.754	20.809
SFG	1.925	0.119	0.005	32.325	26.184
TER	2.924	0.160	0.003	36.443	53.852
AFY	6.780	0.084	0.006	161.626	14.905
BEC	2.097	0.481	0.020	8.723	23.992
BOG	2.528	0.393	0.012	12.855	31.683
MEL	2.594	0.054	0.002	95.872	35.978
MFI	2.748	0.055	0.001	100.558	47.259
ITR	2.321	0.149	0.006	31.163	24.254
SBT	0.968	0.324	0.039	5.980	8.388
STW	4.519	0.037	0.003	247.469	13.430
SZR	2.407	0.036	0.003	133.290	12.950
ITQ-3	3.116	0.259	0.004	24.059	71.405
MTF	1.249	0.047	0.002	52.800	21.257
SAS	2.335	0.415	0.016	11.244	25.918
DDR	1.610	0.133	0.003	24.137	52.881
LEV	1.928	0.367	0.009	10.501	40.805
MWW	2.933	0.264	0.010	22.198	26.446
CHA	2.409	0.369	0.013	13.057	27.801
ERI	2.191	0.252	0.008	17.371	32.525
FAU	0.803	0.278	0.035	5.778	7.925
ITQ-29	2.673	0.384	0.017	13.916	22.950
KFI	2.091	0.397	0.011	10.528	35.640
PAU	2.179	0.191	0.006	22.830	31.904
RHO	1.090	0.310	0.024	7.029	13.069
SBE	1.173	0.228	0.036	10.271	6.430

Table S9. Computed amount of adsorbed molecules and adsorption selectivity from the binary equimolar mixture (CO_2/CO). These values were taken from the adsorption isotherms obtained from Monte Carlo simulations at room conditions for temperature and pressure.

Zeolite	CO_2 loading (mol/kg)	CO loading (mol/kg)	S CO_2/CO	Zeolite	CO_2 loading (mol/kg)	CO loading (mol/kg)	S CO_2/CO
ITW	0.611	0.048	12.787	MTF	0.71	0.013	55.363
JRY	1.127	0.042	27.092	SAS	0.873	0.065	13.469
MOR	0.513	0.094	5.477	DDR	0.946	0.026	36.461
FER	1.451	0.035	41.73	LEV	1.116	0.051	21.68
SFG	0.823	0.034	23.958	MWW	1.148	0.053	21.579
TER	1.241	0.062	20.024	CHA	0.915	0.061	14.923
MEL	1.619	0.034	47.466	FAU	0.255	0.046	5.567
MFI	1.551	0.042	36.63	PAU	0.832	0.047	17.742
STW	1.84	0.06	30.782	RHO	0.384	0.054	7.16
ITQ-3	1.252	0.061	20.45	SBE	0.406	0.059	6.918

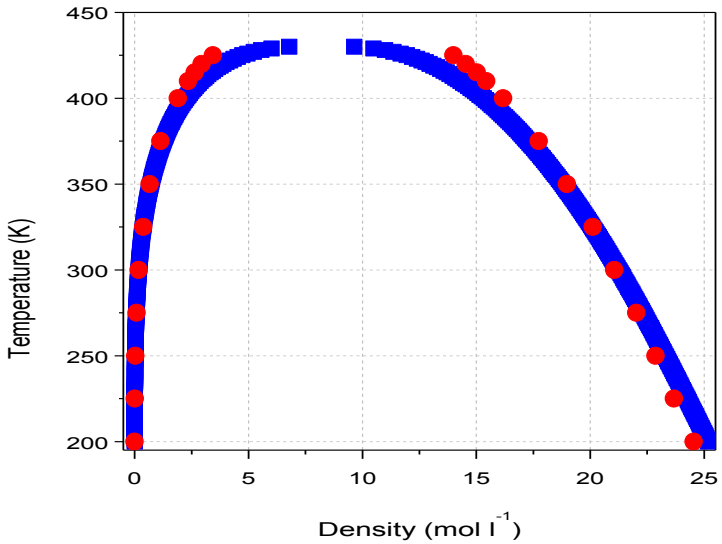
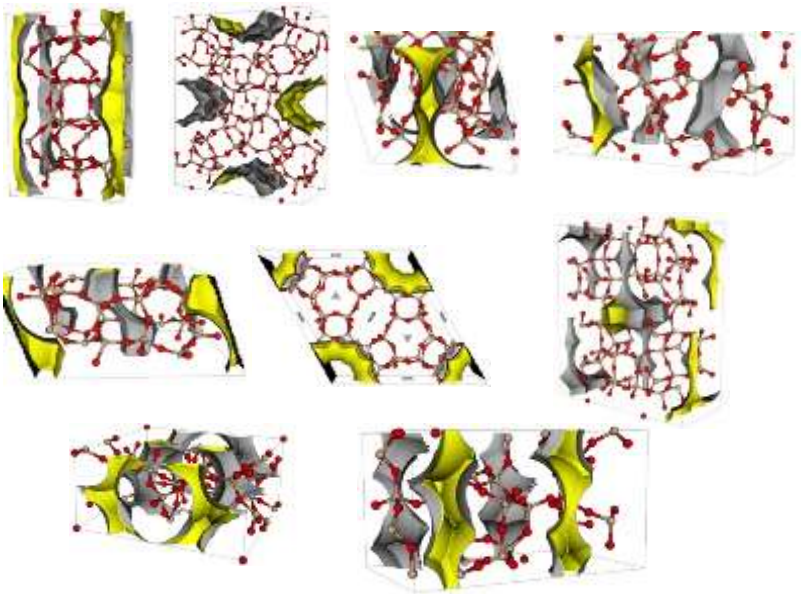


Figure S1. Vapor-liquid equilibrium curve of sulfur dioxide: Comparison of experimental[1] (blue squares) and simulation data (red circles). Note that the force field performs well even near the critical point, where it is well established that Gibbs Ensemble Monte Carlo provides values with large error bars[2].

1D Channels: 1st row: ASV, DON, ITW, JRY; 2nd row: LAU, LTL, MOR; 3rd row: NAT, PON



2D Channels: 1st row: AFR, FER, IWV; 2nd row: NES, SFO, SFG, TER

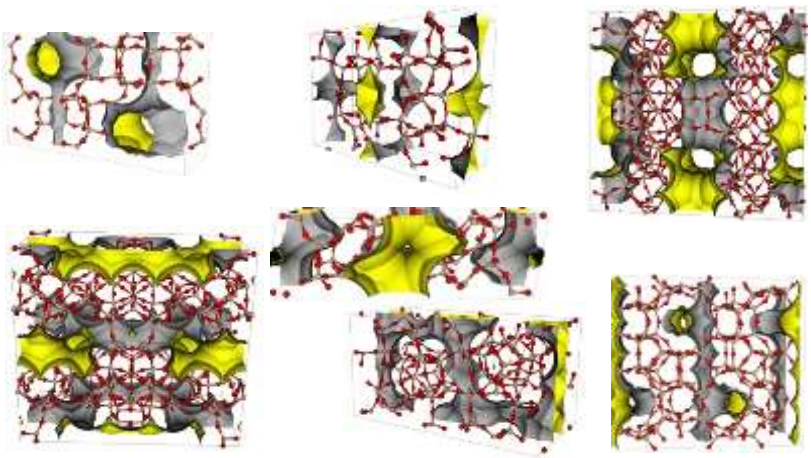


Figure S2. Pore landscapes of the selected 1D and 2D channels-type zeolites. The inner surface of the pores is highlighted in yellow. The color codes for atoms are red and beige for oxygen and silicon, respectively.

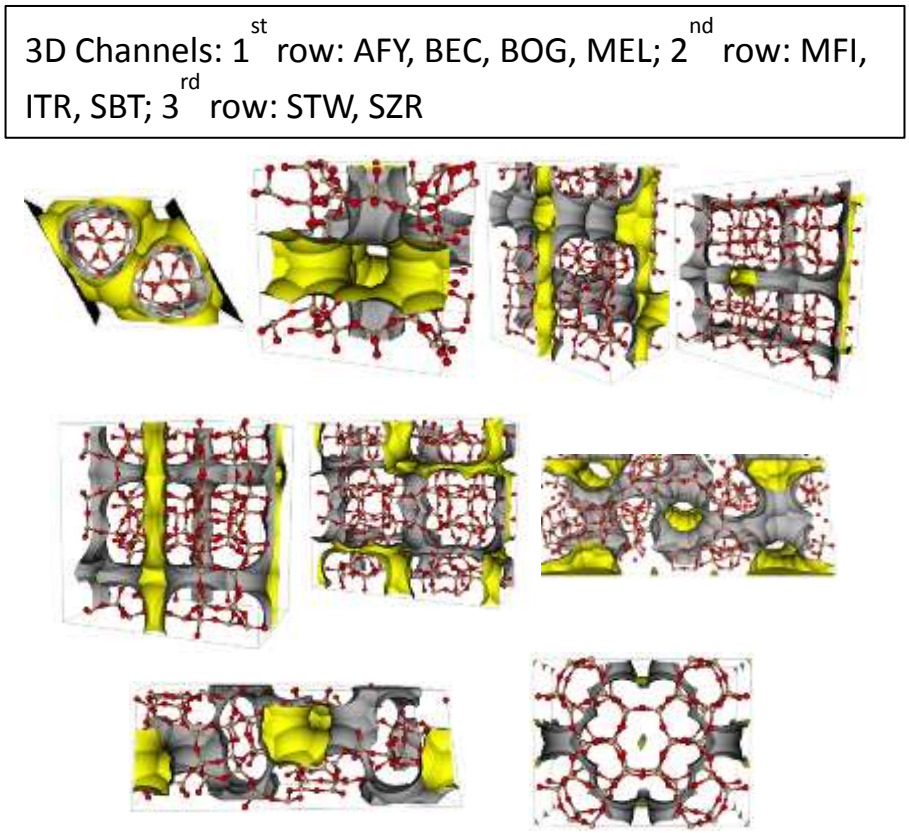


Figure S3. Pore landscapes of the selected 3D channels-type zeolites. The inner surface of the pores is highlighted in yellow. The color codes for atoms are red and beige for oxygen and silicon, respectively.

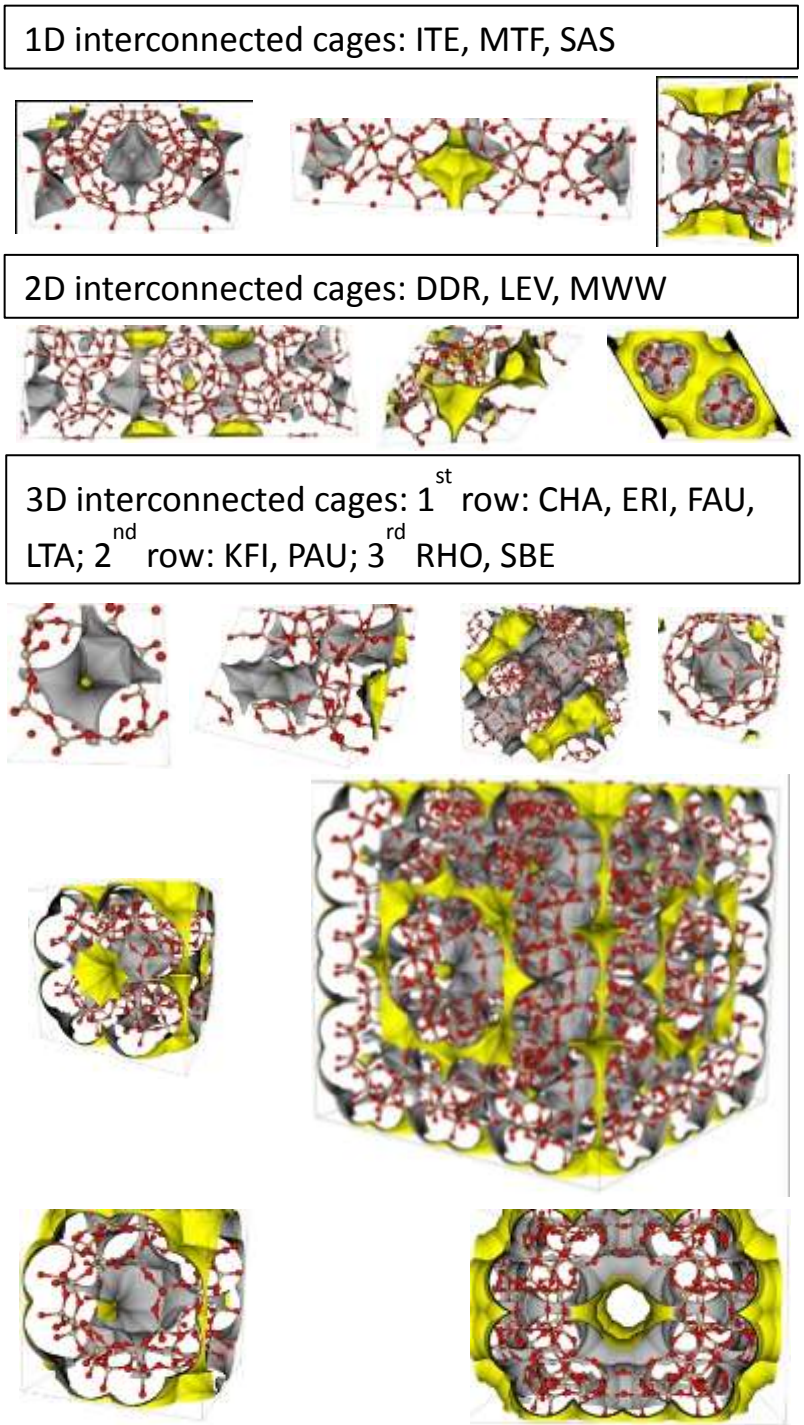


Figure S4. Pore landscapes of the selected zeolites of three considered classes of interconnected cages. The inner surface of the pores is highlighted in yellow. The color codes for atoms are red and beige for oxygen and silicon, respectively.

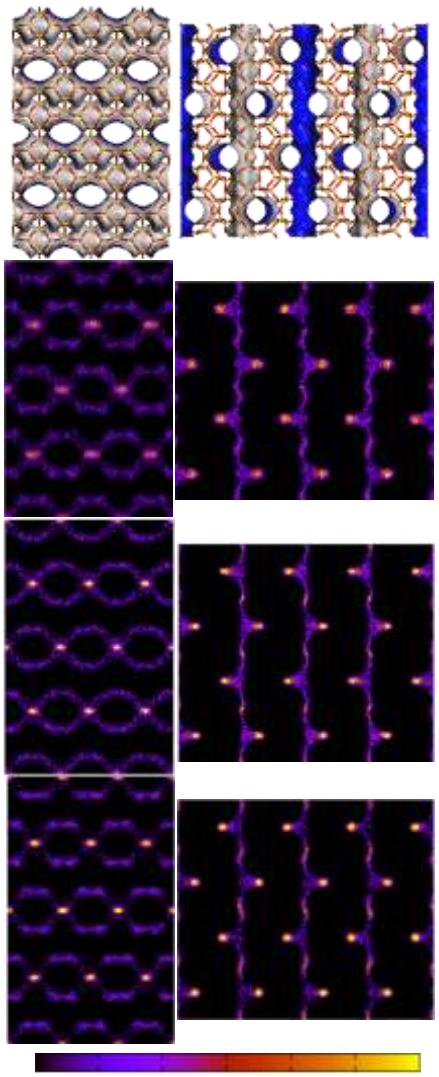


Figure S5. Average occupation profiles of carbon monoxide (second row), carbon dioxide (third row), and sulfur dioxide (fourth row) obtained for one molecule in TER zeolite. The figure shows the projection of the center of mass of the molecules over the x-y (left), and y-z (right) planes. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (first row). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part is colored in blue and the non-accessible part is colored in gray).

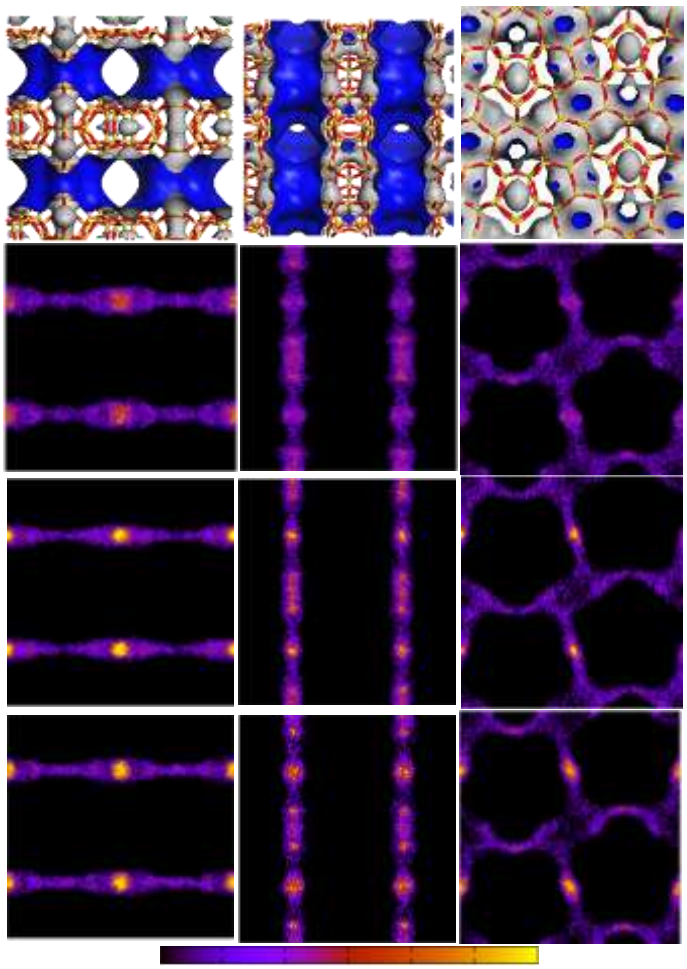


Figure S6. Average occupation profiles of carbon monoxide (second row), carbon dioxide (third row), and sulfur dioxide (fourth row) obtained for one molecule in SFG zeolite. The figure shows the projection of the center of mass of the molecules over the x-y (left), y-z (middle), and x-z (right) planes. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (first row). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part appears in blue and the non-accessible part is colored in gray).

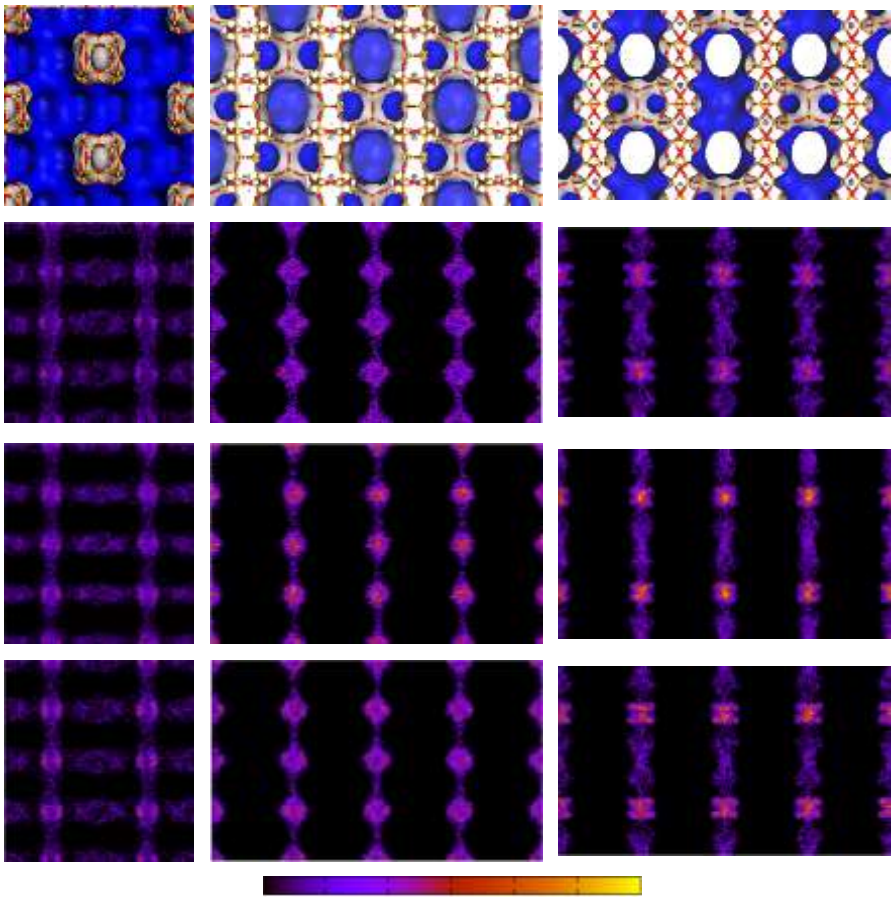


Figure S7. Average occupation profiles of carbon monoxide (second row), carbon dioxide (third row), and sulfur dioxide (fourth row) obtained for one molecule in NES zeolite. The figure shows the projection of the center of mass of the molecules over the x-y (left), z-y (middle), and z-x (right) planes. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (first row). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part appears in blue and the non-accessible part is colored in gray).

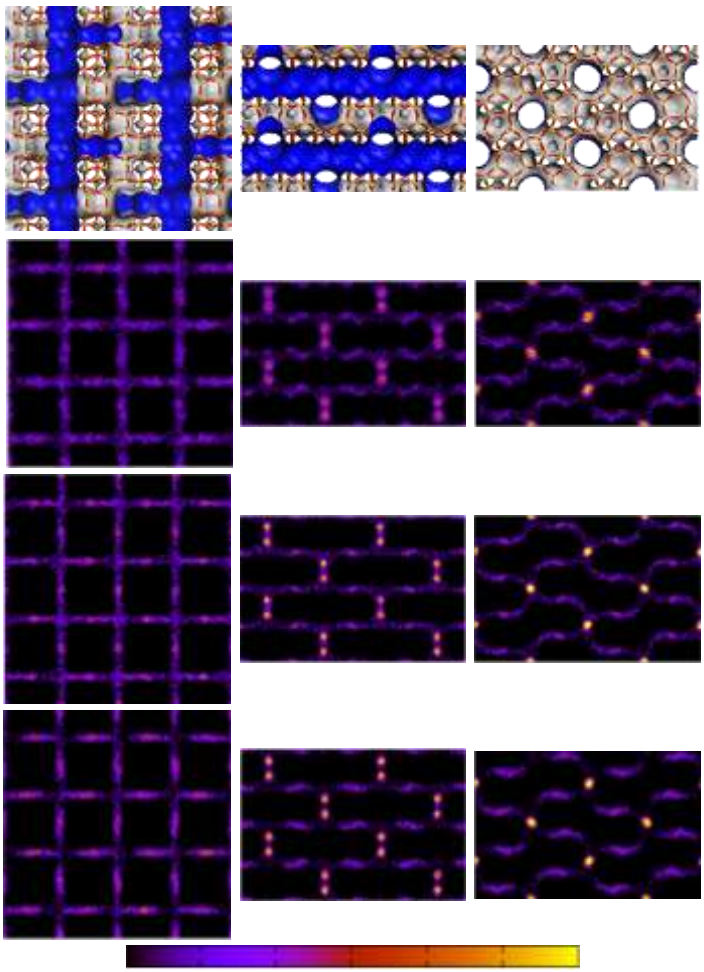


Figure S8. Average occupation profiles of carbon monoxide (second row), carbon dioxide (third row), and sulfur dioxide (fourth row) obtained for one molecule in MFI zeolite. The figure shows the projection of the center of mass of the molecules over the x-y (left), y-z (middle), and x-z (right) planes. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (first row). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part is colored in blue and the non-accessible part is colored in gray).

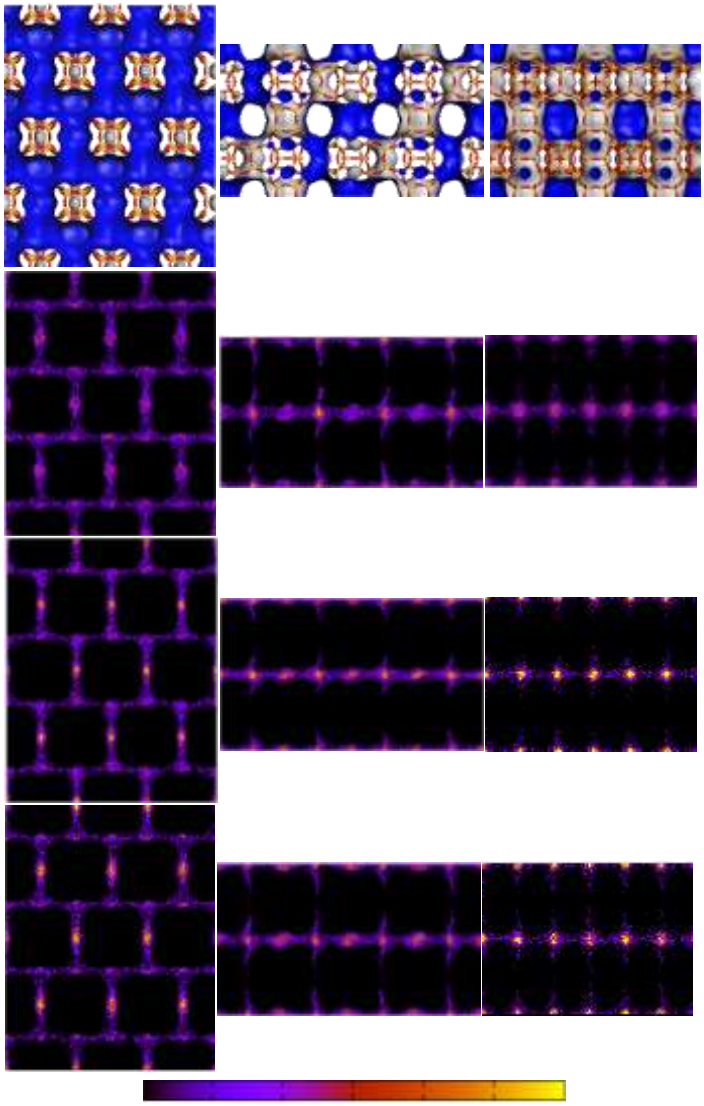


Figure S9. Average occupation profiles of carbon monoxide (second row), carbon dioxide (third row), and sulfur dioxide (fourth row) obtained for one molecule in ITR zeolite. The figure shows the projection of the center of mass of the molecules over the x-y (left), y-z (middle), and x-z (right) planes. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (first row). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part appears in blue and the non-accessible part is colored in gray).

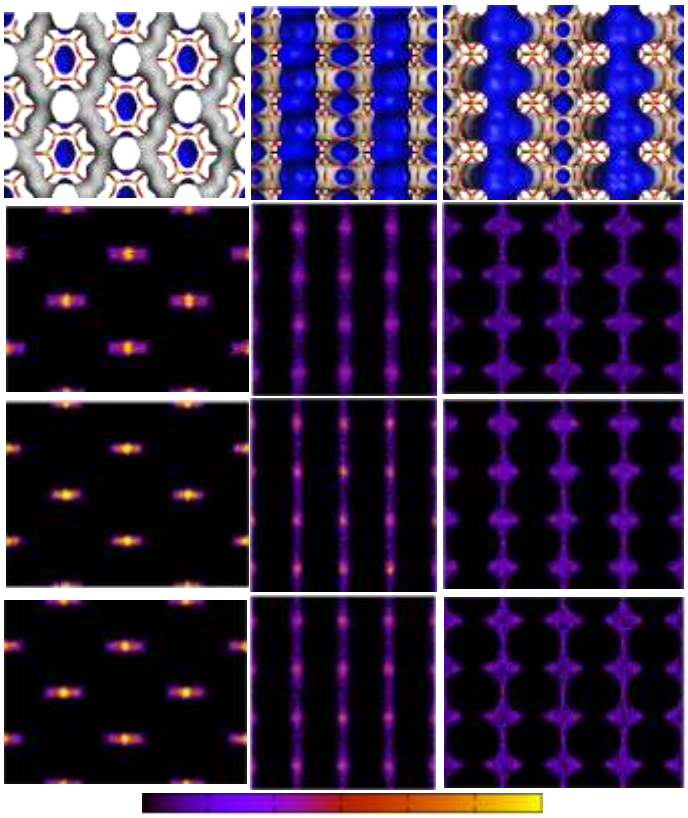


Figure S10. Average occupation profiles of carbon monoxide (second row), carbon dioxide (third row), and sulfur dioxide (fourth row) obtained for one molecule in SZR zeolite. The figure shows the projection of the center of mass of the molecules over the x-y (left), y-z (middle), and x-z (right) planes. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (first row). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part appears in and while the non-accessible part is colored in gray).

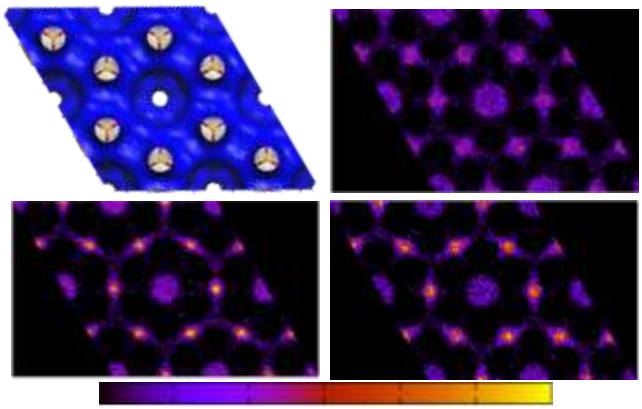


Figure S11. Average occupation profiles of carbon monoxide (top right), carbon dioxide (bottom left), and sulfur dioxide (bottom right) computed for one molecule in MWW zeolite. The figure shows the projection of the center of mass of the molecules over the x-y plane. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (top left). The atomic structure is represented by oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted, where the accessible part appears in blue and the non-accessible part is colored in gray.

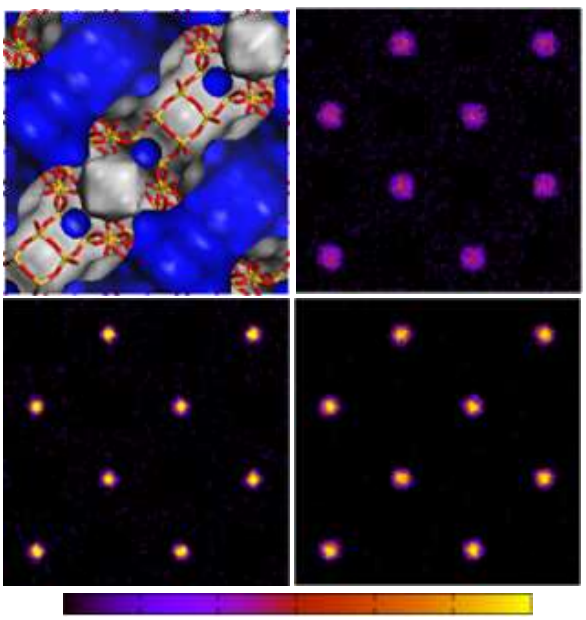


Figure S12. Average occupation profiles of carbon monoxide (top right), carbon dioxide (bottom left), and sulfur dioxide (bottom right) computed for one molecule in FAU zeolite. The figure shows the projections of the center of mass of the molecules over the x-y plane. The color graduation indicates the occupational density (from black to yellow). To guide the view we add a representation of the structure (top left). The atomic structure is represented by the oxygen and silica atoms in red and yellow respectively. A grid surface is also depicted (where the accessible part is colored in blue and the non-accessible part is colored in gray).

Notes and references

1. National Institute of Standards and Technology, http://www.nist.gov/index.html, Accessed January, 2013.
2. A. Z. Panagiotopoulos, Gibbs ensemble techniques, 1995.