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

ZEOLITES FOR THE SELECTIVE ADSORPTION OF SULFUR HEXAFLUORIDE

I. Matito-Martos[a], J. Álvarez-Ossorio[a], J.J. Gutiérrez-Sevillano[a], M. Doblaré[b], A. Martin-Calvo*[a], and S. Calero*[a]

Department of Physical, Chemical and Natural Systems, University Pablo de Olavide, Sevilla 41013, Spain
Abengoa Research, Abengoa, Campus Palmas Altas, Energía Solar, 1. (Palmas Altas) 41014 Seville, Spain

Electronic Supporting Information

Table S1. Unit cell lengths and angles, and computed pore volume, and surface area for the zeolites used in this study.

Zeolite	Crystallographic Positions	Unit cell a (Å)	Unit cell b (Å)	Unit cell c (Å)	Angles unit cell a (°)	Angles unit cell b (°)	Angles unit cell g (°)	Pore Volume (cm^3/g)	SSA (Helium) (m^2/g)
AFR	1	22.31	13.57	6.97	90	90	90	0.249	818.00
AFY	1	12.33	12.33	8.60	90	90	120	0.295	1208.05
ASV	1	8.67	8.67	13.92	90	90	90	0.096	305.30
BEC	1	12.77	12.77	12.98	90	90	90	0.284	979.93
BOG	2	20.24	23.80	12.80	90	90	90	0.240	817.50
CFI	1	13.96	5.26	25.97	90	90	90	0.149	456.56
CHA	3	9.46	9.46	9.46	94.07	94.07	94.07	0.253	893.81
DDR	4	13.86	13.86	40.89	90	90	120	0.140	400.48
DON	5	14.97	8.48	30.03	90	102.65	90	0.167	508.77
EMT	1	17.22	17.22	28.08	90	90	120	0.340	1030.19
EON	1	7.57	18.15	25.93	90	90	90	0.164	378.34
ERI	6	13.27	13.27	15.05	90	90	120	0.219	716.96
FAU	7	24.26	24.26	24.26	90	90	90	0.332	1020.96
FER	8	18.72	14.07	7.42	90	90	90	0.129	407.45
ITQ-29	9	11.87	11.87	11.87	90	90	90	0.286	849.36
ITQ-3	10	20.62	9.72	19.62	90	90	90	0.227	693.71
ITR	1	11.67	21.97	25.17	90	90	90	0.155	572.09
ITW	1	10.45	15.03	8.95	90	105.64	90	0.102	382.27
IWW	1	41.69	12.71	12.71	90	90	90	0.197	883.36
JRY	1	8.17	9.20	17.29	90	90	90	0.094	333.56
KFI	11	18.67	18.67	18.67	90	90	90	0.233	786.75
LAU	12	14.85	13.17	7.54	90	110.323	90	0.133	471.29
LEV	13	13.34	13.34	23.01	90	90	120	0.219	706.26
LTL	14	18.47	18.47	7.48	90	90	120	0.168	553.03
MEL	15	20.07	20.07	13.41	90	90	90	0.154	544.96
MFI	16	20.02	19.90	13.38	90	90	90	0.164	547.66
MOR	17	18.11	20.53	7.53	90	90	90	0.150	477.93
MTF	1	9.63	30.39	7.25	90	90.45	90	0.086	263.69
MWW	1	14.39	14.39	25.20	90	90	120	0.233	801.23
NES	1	26.06	13.88	22.86	90	90	90	0.194	701.99
OBW	1	13.91	13.91	30.84	90	90	90	0.324	989.06
PAU	18	35.09	35.09	35.09	90	90	90	0.159	538.21
PON	1	8.91	9.21	16.09	90	90	90	0.094	329.22
RHO	19	15.03	15.03	15.03	90	90	90	0.252	783.40
SAS	1	14.35	14.35	10.40	90	90	90	0.259	794.61
SBE	1	18.53	18.53	27.13	90	90	90	0.307	938.11
SBT	1	17.19	17.19	41.03	90	90	120	0.339	1057.79
SFG	1	25.53	12.58	13.07	90	90	90	0.141	494.75
SFO	1	22.59	13.57	6.97	90	99.016	90	0.249	815.75
STW	1	11.89	11.89	29.92	90	90	120	0.203	804.89
SZR	1	18.87	14.40	7.51	90	90	90	0.117	398.51
TER	1	9.81	23.65	20.24	90	90	90	0.176	647.26

Table S2.Self-diffusion coefficients calculated for sulfur hexafluoride in the studied zeolites. Simulations carried out at 298 K with two molecules per simulation cell.

Zeolite	D_{avg} (10^{-8} m^2 s^{-1})	D_X (10^{-8} m^2 s^{-1})	D_y (10^{-8} m^2 s^{-1})	D_z (10^{-8} m^2 s^{-1})	Zeolite	D_{avg} (10^{-8} m^2 s^{-1})	D_X (10^{-8} m^2 s^{-1})	D_y (10^{-8} m^2 s^{-1})	D_z (10^{-8} m^2 s^{-1})
AFR	0.2031	-	-	0.6100	**LAU**	-	-	-	-
AFY	0.2594	-	-	0.7735	**LEV**	-	-	-	-
ASV	-	-	-	-	**LTL**	0.0666	-	-	0.1969
BEC	0.2736	0.3703	0.3663	0.1026	**MEL**	0.0008	0.0010	0.0010	0.0005
BOG	0.2892	0.8453	0.0199	-	**MFI**	0.0302	0.0300	0.0564	0.0114
CFI	0.8558	-	2.5671	-	**MOR**	0.8245	-	-	2.4735
CHA	-	-	-	-	**MTF**	-	-	-	-
DDR	-	-	-	-	**MWW**	-	-	-	-
DON	0.6025	-	1.8065	-	**NES**	0.0161	0.0374	0.0128	-
EMT	0.4793	0.4416	0.4478	0.5366	**OBW**	0.0050	0.0082	0.0049	-
EON	0.6589	1.9769	-	-	**PAU**	-	-	-	-
ERI	-	-	-	-	**PON**	-	-	-	-
FAU	0.8132	0.8276	0.8319	0.8030	**RHO**	-	-	-	-
FER	-	-	-	-	**SAS**	-	-	-	-
LTA	-	-	-	-	**SBE**	0.2557	0.3845	0.3788	-
ITE	-	-	-	-	**SBT**	0.4124	0.4659	0.4490	0.3164
ITR	0.0012	0.0007	0.0002	0.0028	**SFG**	0.0049	-	-	0.0148
ITW	-	-	-	-	**SFO**	0.1957	0.0117	-	0.5743
IWW	0.0313	-	-	0.0993	**STW**	0.0029	-	-	0.0088
JRY	-	-	-	-	**TER**	0.0240	0.0719	-	-
KFI	-	-	-	-	**-**	-	-	-	-

Table S3. Loading of SF_6 and N_2 and SF_6/N_2 selectivity at the given pressure from the mixture SF_6/N_2 (10:90) at room temperature. The values of pressure were chosen using criteria that combines both high selectivity and SF_6 loading.

Zeolite	Pressure kPa	SF_6 Loading mol/kg	N_2 Loading mol/kg	Selectivity SF_6/N_2
AFR	300	1.07	0.20	48.39
AFY	300	0.61	0.34	16.31
BEC	300	2.28	0.07	296.06
BOG	300	1.53	0.17	80.74
CFI	300	0.68	0.08	80.25
DON	300	0.55	0.11	43.30
EMT	3000	2.28	0.74	27.61
EON	60	0.35	0.04	74.76
FAU	1000	1.52	0.50	27.64
ITR	300	1.73	0.02	731.10
IWW	300	1.70	0.04	404.12
LTL	1000	1.22	0.27	40.60
MEL	300	1.80	0.11	144.01
MFI	300	1.75	0.11	145.69
MOR	60	0.58	0.08	61.70
NES	300	1.43	0.08	151.24
OBW	300	0.57	0.18	27.79
SBE	1000	1.40	0.64	19.68
SBT	3000	2.93	0.54	48.81
SFG	300	1.28	0.04	327.16
SFO	300	1.68	0.09	169.06
STW	300	0.51	0.52	8.84
TER	100	0.82	0.13	56.17

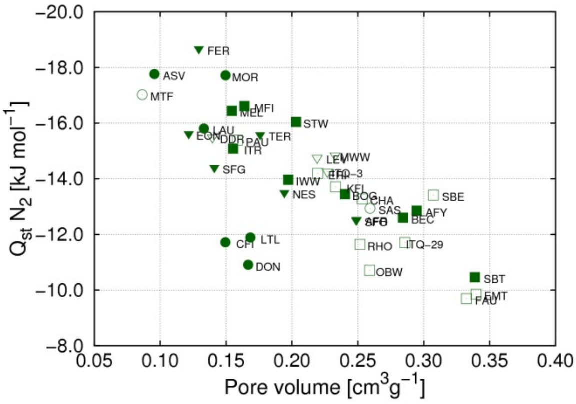

Figure S1. Computed isosteric heats of adsorption of sulfur hexafluoride at 298 K as a function of the zeolite pore volume. Open symbols show the results obtained for channel-type zeolites and closed symbol for the interconnected-type. The directionally of the pore space is represented by circles (1D), inverted triangles (2D), and squares (3D).

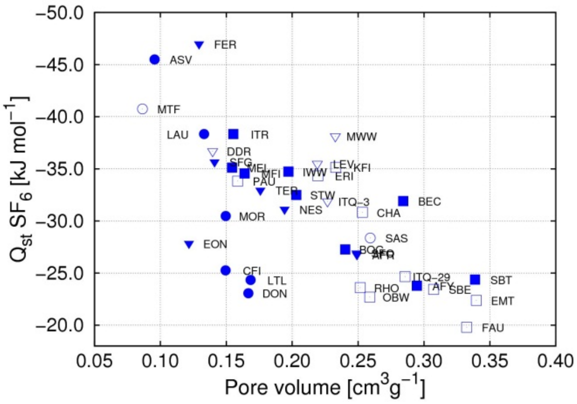

Figure S2. Computed isosteric heats of adsorption of sulfur hexafluoride at 298 K as a function of the zeolite pore volume. Open symbols show the results obtained for channel-type zeolites and closed symbol for the interconnected-type. The directionally of the pore space is represented by circles (1D), inverted triangles (2D), and squares (3D).

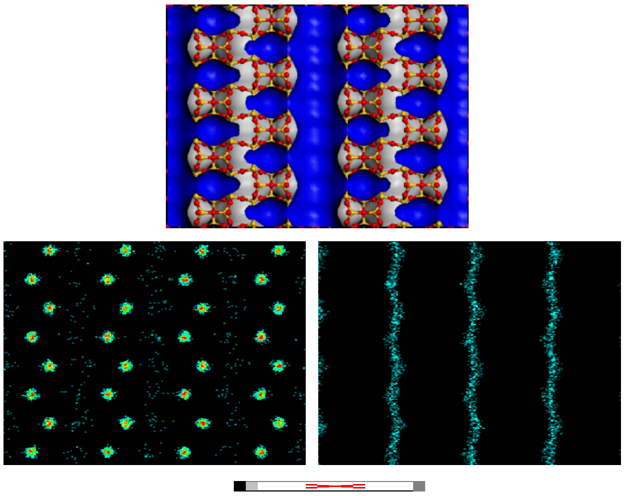

Figure S3. Average occupation profiles obtained in MOR zeolite for nitrogen (bottom left) and sulfur hexafluoride (bottom right). These figures show the projection of the center of mass of the molecules over the *z-x* plane. The color graduation indicates the occupation density (from black to red). To guide the view we add a representation of the structure (top). Oxygen atoms are depicted in red and silica atoms in yellow. A grid surface is also represented where the accessible part appears in blue while the non-accessible part is colored in gray.

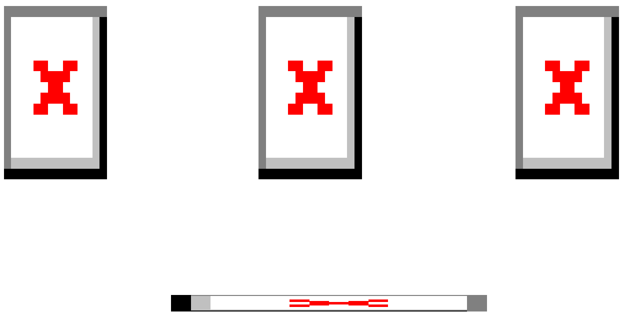

Figure S4. Average occupation profiles obtained in EON zeolite for nitrogen (center) and sulfur hexafluoride (right). These figures show the projection of the center of mass of the molecules over the *z-x* plane. The color graduation indicates the occupation density (from black to red). To guide the view we add a representation of the structure (left). Oxygen atoms are depicted in red and silica atoms in yellow. A grid surface is also represented where the accessible part appears in blue while the non-accessible part is colored in gray.

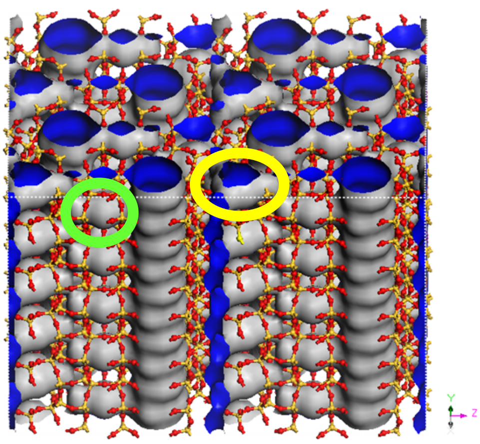

Figure S5. Representation of the atomic structure of zeolite EON. Oxygen atoms are depicted in red and silica atoms in yellow. A grid surface is also represented where the accessible part appears in blue while the non-accessible part is colored in gray. Local structure features are highlighted with circles colored in green (side-pockets) and yellow (T-box).

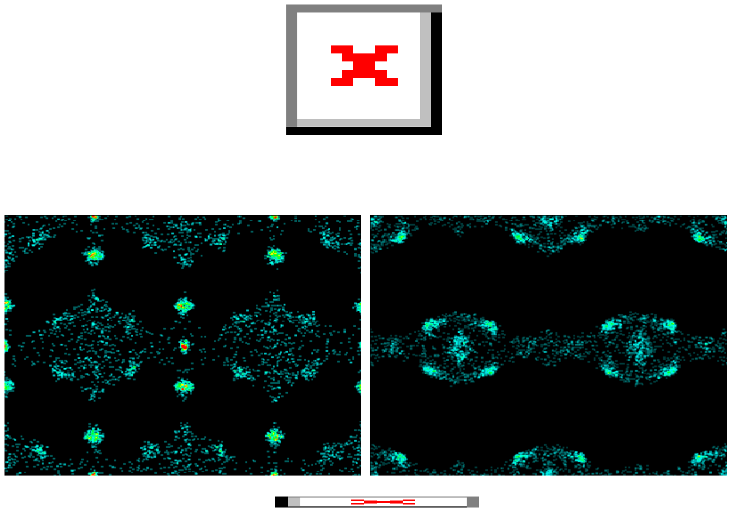

Figure S6. Average occupation profiles obtained in SBE zeolite for nitrogen (bottom left) and sulfur hexafluoride (bottom right). These figures show the projection of the center of mass of the molecules over the *z-x* plane (or *y-z* plane). The color graduation indicates the occupation density (from black to red). To guide the view we add a representation of the structure (top). Oxygen atoms are depicted in red and silica atoms in yellow. A grid surface is also represented where the accessible part appears in blue while the non-accessible part is colored in gray.

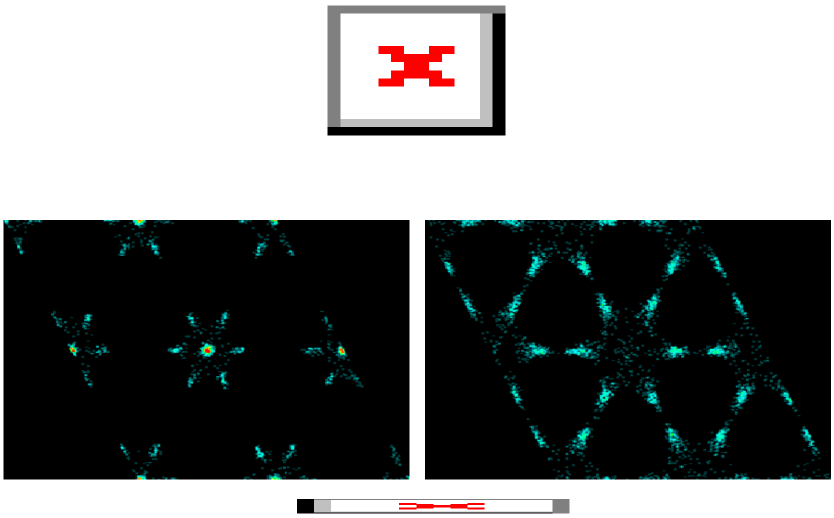

Figure S7. Average occupation profiles obtained in AFY zeolite for nitrogen (bottom left) and sulfur hexafluoride (bottom right). These figures show the projection of the center of mass of the molecules over the *x-y* plane. The color graduation indicates the occupation density (from black to red). To guide the view we add a representation of the structure (top). Oxygen atoms are depicted in red and silica atoms in yellow. A grid surface is also represented where the accessible part appears in blue while the non-accessible part is colored in gray.

References and Notes

1. C. Baerlocher, L. B. McCusker and D. H. Olson, *Atlas of Zeolite Framework types*, Elsevier, London, 2007.
2. J. J. Pluth and J. V. Smith, *Am. Miner.*, 1990, **75**, 501-507.
3. M. Calligaris, G. Nardin and L. Randaccio, *Zeolites*, 1983, **3**, 205-208.
4. H. Gies, *Z. Kristallogr.*, 1986, **175**, 93-104.
5. T. Wessels, C. Baerlocher, L. B. McCusker and E. J. Creyghton, *Journal of the American Chemical Society*, 1999, **121**, 6242-6247.
6. J. A. Gard and J. M. Tait, *Proc. 3rd Int. Conf. Molecular Sieves*, 1973, 94-99.
7. J. A. Hriljac, M. M. Eddy, A. K. Cheetham, J. A. Donohue and G. J. Ray, *J. Solid State Chem.*, 1993, **106**, 66-72.
8. R. E. Morris, S. J. Weigel, N. J. Henson, L. M. Bull, M. T. Janicke, B. F. Chmelka and A. K. Cheetham, *Journal of the American Chemical Society*, 1994, **116**, 11849-11855.
9. A. Corma, F. Rey, J. Rius, M. J. Sabater and S. Valencia, *Nature*, 2004, **431**, 287-290.
10. M. A. Camblor, A. Corma, P. Lightfoot, L. A. Villaescusa and P. A. Wright, *Angewandte Chemie-International Edition*, 1997, **36**, 2659-2661.
11. J. B. Parise, R. D. Shannon, E. Prince and D. E. Cox, *Z. Kristall.*, 1983, **165**, 175-190.
12. G. Artioli and K. Stahl, *Zeolites*, 1993, **13**, 249-255.
13. S. Merlino, E. Galli and A. Alberti, *Tschermaks Min. Petr. Mitt*, 1975, **22**, 117-129.
14. J. M. Newsam, *J. Phys. Chem.*, 1989, **93**, 7689-7694.
15. C. A. Fyfe, H. Gies, G. T. Kokotailo, C. Pasztor, H. Strobl and D. E. Cox, *Journal of the American Chemical Society*, 1989, **111**, 2470-2474.
16. H. van Koningsveld, H. van Bekkum and J. C. Jansen, *Acta Crystallogr. Sect. B-Struct. Commun.*, 1987, **43**, 127-132.
17. V. Gramlich, Ph.D. Thesis, ETH, Zürich, Switzerland, 1971.
18. E. K. Gordon, S. Samson and W. B. Kamb, *Science*, 1966, **154**, 1004-1007.
19. L. B. McCusker and C. Baerlocher, *J. Solid State Chem.*, 1984, 812-822.