Electronic Supplementary Material (ESI) for Chemical Society Reviews

Simulating the Properties of Small Pore Silica Zeolites Using Interatomic Potentials

Electronic Suplementary Information

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1 Force Fields, FFs, selected for the study.

Potentials in Table 1 are classified according to: a) parametrization method; b) data source for the parametrization; c) if polarizability is explicitly included via the shell model, the QEq or FQ models; d) if the atoms bears formal or partial charges. This work does not intend to show the details of the process of developing FFs, but rather to show their ability to reproduce and predict particular properties of several silica materials, so we refer the reader to the original references (See Table 1) for in depth information. A complete set of parameters is provided in ESI (section 2, Tables 2-4) for all of the models studied.

Table 1: FFs, references, parametrization method, polarizability method and applications.

FF and Reference		**Parametrization / Data Source**	**Polarizability**
Sanders *et al.* [1]	***SLC***	Empirical ($\alpha - quartz$)	FC / SM
Schröeder and Sauer [2]	***SS96***	*Ab initio* ($SiO_4, AlO_4 - Tetrahedra$)	FC / SM
Sierka and Sauer [3]	***SS97***	*Ab initio (4-6 aluminosilicate rings)*	FC / SM
Gale [4]	***Gale***	Empirical ($\alpha - quartz$)	FC / SM
Sastre and Corma [5]	***SC1***	Empirical ($\alpha - quartz$)	FC / SM
Pedone *et al.* [6]	***PMM08***	Periodic DFT	PC / SM
Jackson and Catlow [7]	***JC***	Empirical ($\alpha - quartz$)	FC / RI
Demontis *et al.* [8]	***DSQFG***	Empirical (Natrolite, Zeolites)	FC / RI
Jaramillo and Auerbach [9]	***JA***	*Ab initio* / Empirical ($\alpha - quartz$)	PC / RI
Auerbach *et al.* [10]	***AHCM***	*Ab initio* / Empirical ($\alpha - quartz$)	PC / RI
Van Beest *et al.* [11]	***BKS***	*Ab initio* / Empirical ($\alpha - quartz$)	PC / RI
Vessal [12]	***Vessal***	Empirical ($\alpha - quartz$)	FC / RI
Pedone *et al.* [13]	***PMM06***	Empirical (Different Crystal Structures)	PC / RI
Tsuneyuki *et at.* [14]	**TTAM**	*Ab initio* / ($\alpha - quartz$)	PC / RI
Sastre and Corma [5]	***SC2***	Empirical ($\alpha - quartz$)	FC / MM
Smirnov and Bougeard [15]	**SB**	-	MM

FC=Formal Charge, SM=Shell Model, PC=Partial Charge, RI=Rigid Ion.

2 8-ring zeolites

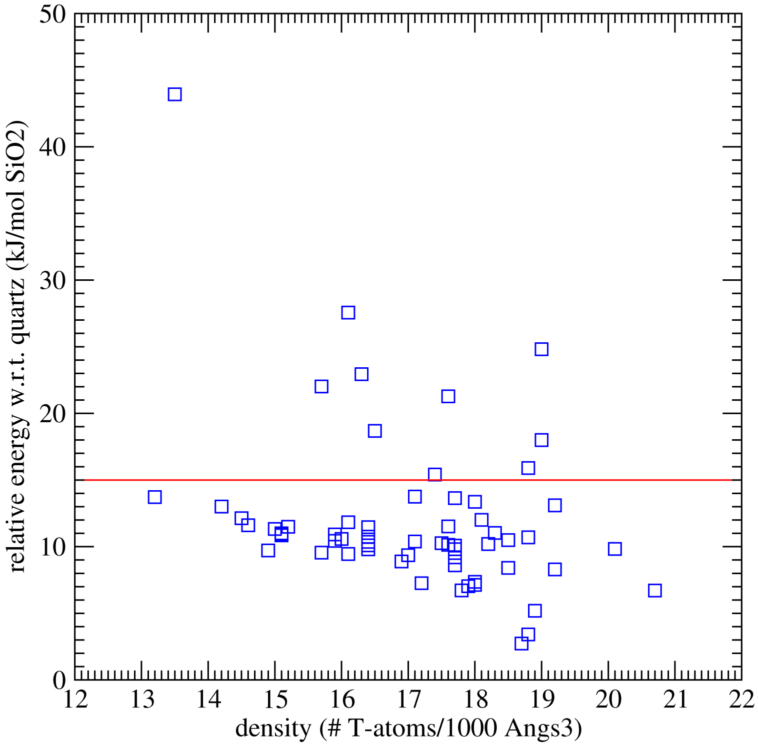
Table 2: List of the 64 zeotypes belonging to the Atlas of Zeolite Framework Types (as of May-2012, [16]) containing 8-rings as the largest window. The density has been calculated in the pure silica composition, and its corresponding energy with respect to quartz has been calculated according to a recent study [17]. A plot of density vs. energy is shown in Figure 1.

#	Code	Name	density (Si/1000 A^{a})	Dim	Energy (kJ/mol SiO_2)
1	ABW	Li-A	17.6	1	11.52
2	ACO	ACP-1	16.5	3	18.68
3	AEI	AlPO-18	15.1	3	11.00
4	AEN	AlPO-EN3	20.1	2	9.83
5	AFN	AlPO-14	17.4	3	15.41
6	AFT	AlPO-52	15.1	3	10.90
7	AFX	SAPO-56	15.1	3	10.92
8	ANA	Analcime	19.2	3	8.29
9	APC	AlPO-C	17.7	2	13.64
10	APD	AlPO-D	18.0	2	7.36
11	ATN	MAPO-39	17.8	1	6.72
12	ATT	AlPO-12-TAMU	17.1	2	10.39
13	ATV	AlPO-25	18.9	1	5.19
14	AWO	AlPO-21	18.2	1	10.20
15	AWW	AlPO-22	16.9	1	8.89
16	BCT	Mg-BCTT	19.0	1	24.81
17	BIK	Bikitaite	18.7	1	2.73
18	BRE	Brewsterite	18.3	2	11.03
19	CAS	Cesium	18.8	1	3.41
20	CDO	CDS-1	18.1	2	12.01
21	CHA	Chabazite	15.1	3	10.85
22	DDR	Deca-dodecasil 3R	17.9	2	7.04
23	DFT	DAF-2	17.7	3	9.81
24	EAB	TMA-E	16.0	2	10.58
25	EDI	Edingtonite	16.3	3	22.94
26	EPI	Epistilbite	17.7	2	9.20
27	ERI	Erionite	16.1	3	11.83
28	ESV	ERS-7	17.7	1	8.60
29	GIS	Gismondine	16.4	3	9.80
30	GOO	Goosecreekite	19.0	3	18.00
31	IHW	ITQ-32	18.5	2	8.41
32	ITE	ITQ-3	15.7	2	9.55
33	ITW	ITQ-12	17.7	2	10.08
34	JBW	Na-J	18.8	1	10.70
35	KFI	ZK-5	15.0	3	11.33
36	LEV	Levyne	15.9	2	10.43
37	-LIT	Lithosite	19.2	0	
38	LTA	Linde type A	14.2	3	13.01
39	LTJ	Linde type J	18.5	2	10.49
40	LTN	Linde type N	17.0	0	9.36

Table 1. (Continuation)

#	Code	Name	density (Si/1000 A3)	Dim	Energy (kJ/mol SiO_2)
41	MER	Merlinoite	16.4	3	10.75
42	MON	Montesommaite	17.6	2	10.14
43	MTF	MCM-35	20.7	1	6.71
43	NPT	Oxonitridophosphate-2	13.5	3	43.94
45	NSI	Nu-6(2)	18.8	2	15.90
46	OWE	UiO-28	17.1	2	13.75
47	PAU	Paulingite	15.9	3	10.92
48	PHI	Phillipsite	16.4	3	10.36
49	RHO	Rho	14.5	3	12.13
50	RTE	RUB-3	17.2	1	7.26
51	RTH	RUB-13	16.1	2	9.45
52	RWR	RUB-24	19.2	1	13.10
53	SAS	STA-6	14.9	1	9.71
54	SAT	STA-2	16.4	3	11.46
55	SAV	Mg-STA-7	14.6	3	11.61
56	SBN	UCSB-9	16.1	3	27.56
57	SIV	SIZ-7	16.4	3	10.10
58	THO	Thomsonite	15.7	3	22.02
59	TSC	Tschörtnerite	13.2	3	13.72
60	UEI	Mu-18	17.5	2	10.26
61	UFI	UZM-5	15.2	2	11.49
62	VNI	VPI-9	17.6	3	21.28
63	YUG	Yugawaralite	18.0	2	7.13
64	ZON	ZAPO-M1	18.0	2	13.37

Figure 1: Plot of energy (with respect to quartz) versus density corresponding to the pure silica zeolites indicated in Table 2. Structures below 15 kJ/mol SiO_2 are considered to be stable as pure silica composition according to a previous study [17]. 53 out of 64 structures are below such threshold.



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3 Force fields parameters

Table 3: Rigid Ion FF Parameters.

	BKS	*TTAM*	*AHCM*	*JA*	Vessal	*JC*	PMM06
Charges							
Si_c[e]	+2.4	+2.4	+2.4	+2.05	+4.0	+4.0	+2.4
O_c[e]	-1.2	-1.2	-1.2	-1.025	-2.0	-2.0	-1.2
Buckingham							
A_{Si-O}[eV]	18003.7572	10703.0000	17796.1	17796.1	1005.1563	1584.167	
A_{O-O}[eV]	1388.7730	1753.8000	1305.9	1305.9	4978496.9	22764.0	
A_{Si-Si}[eV]		8.61588E+8					
ρ_{Si-O} [Å]	0.205205	0.208510133	0.2049	0.2049	0.3277	0.32962	
ρ_{O-O}[Å]	0.362319	0.353805711	0.3594	0.3594	0.149	0.149	
ρ_{Si-Si} [Å]		0.0657					
C_{Si-O} [eVÅ^6]	133.5381	70.6100	135.4	135.4	25.0	52.64511	
C_{O-O}[eVÅ^6]	175.0000	214.3700	196.1	196.1	52.12	27.88	
C_{Si-Si} [eVÅ^6]		23.2603					
Morse							
D_e[eV]							0.340554
a_{si-O}[Å^{-2}]							2.006700
r_{Si-0}[Å]							2.100000
D_e[eV]							0.042395
a_{O-O}[Å^{-2}]							1.379316
r_{O-O}[Å]							3.618701
D_e[eV]							
a_{Si-Si}[Å^{-2}]							
r_{Si-Si}[Å]							
Buckingham 4							
$r_1[Si-O/O-O]$[Å]					1.5 / 2.9		
$r_2[Si-O/O-O]$[Å]					2.5 / 3.6		
$r_3[Si-O/O-O]$[Å]					3.5 / 4.2		
$r_4[Si-O/O-O]$[Å]					7.6 / 7.6		
Vessal							
$K_{O-[Si]-O}$[eV/**rad**^{2}]			729.0189	729.0189	729.0189		
ρ_1 [Å]			0.3277	0.3277	0.3277		
ρ_2 [Å]			0.3277	0.3277	0.3277		
θ_0[**rad**]			109.47	109.47	109.47		
Harmonic							
$Si-O$[ev/Å^2]							
ρ_{Si-O} [Å]							
Harmonic Three							
K_{O-Si-O}[eV/**rad**^{2}]						4.5815	
θ_0						109.47	

Table 4: Shell Model FF Parameters.

	SLC	*SS96*	*SS97*	*Gale*	SC1	PMM08
Charges						
Si_c [e]	+4.0	+4.0	+4.0	+4.0	+4.0	+2.722600
O_c [e]	+0.8482	+1.06237	+1.22858	+0.86902	+0.86902	+1.919810
O_s [e]	-2.8482	-3.06237	-3.22858	-2.86092	-2.86092	-3.281110
Shell - Spring						
O_c-O_s [eV/$\mathbf{Å}^2$]	74.9204	112.7629	122.47853	79.074	74.92	256.71027
Buckingham						
A_{Si-O} [eV]	1283.9073	1550.950	1612.45920	1277.514	1824.2944	8166.2632
A_{O-O} [eV]	22764.000			22764.00	2046.0422	15039.909
ρ_{Si-O} [$\mathbf{Å}$]	0.32052	0.30017	0.29955	0.32052	0.289798	0.193884
ρ_{O-O} [$\mathbf{Å}$]	0.14900			0.14900	0.134015	0.227708
C_{Si-O} [eV$\mathbf{Å}^6$]	10.6616			5.9062	0.00	0.00
C_{O-O} [eV$\mathbf{Å}^6$]	27.879			27.879	14.027	0.00
Urey Bradley						
K_{O-Si-O} [eV/$\mathbf{Å}^2$]				2.30273		
r_0 [$\mathbf{Å}$]				2.43352		
Harmonic Three						
K_{O-Si-O} [eV/$\mathbf{rad}^2$]	2.097	0.18397	0.144703		2.0972	
θ_0	109.47	109.47	109.47		109.47	
Vessal						
$K_{Si-[O]-Si}$ [eV/$\mathbf{rad}^2$]					729.0189	
ρ_1 [$\mathbf{Å}$]					0.3277	
ρ_2 [$\mathbf{Å}$]					0.3277	
θ_0 [$\mathbf{rad}$]					109.47	

Table 5: Molecular Mechanics FF Parameters.

	DSQFG	SC2	SB
Charges			
Si_c [e]	+4.0	+0.0	
O_c [e]	-2.0	+4.24	
O_s [e]		-4.24	
Shell - Spring			
O_c-O_s [eV/Å^2]		74.92	
Harmonic Two			
K_{Si-O} [eV/Å^2]	21.68	58.9576	25.90
r_0^{Si-O} [Å]	1.605	1.605	1.61
Urey Bradley			
K_{O-Si-O} [eV/Å^2]	4.4666		
r_0 [Å]	2.618		
Harmonic Three			
K_{O-Si-O} [eV/rad^2]		6.00	5.99
θ_{O-Si-O}		109.47	109.47
$K_{Si-O-Si}$ [eV/rad^2]			0.79
$\theta_{Si-O-Si}$			142
Vessal			
$K_{Si-[O]-Si}$ [eV/rad^2]		4633.8	
ρ_1 [Å]		0.400	
ρ_2 [Å]		0.400	
θ_0 [rad]		145.00	

4 Structural properties of silica polymophs

Table 6: α,β-Quartz and Coesite: lattice parameters and cell volume.

Structure	a [Å]	b [Å]	c [Å]	$\alpha/\beta/\gamma$ [rad]	Vol [Å^3]
α-Quartz [18]	4.92	4.91	5.40	90/90/120	113.1
β-Quartz[18, 19]	5.00	5.00	5.46	90/90/120	118.0
Coesite[20]	7.147	12.383	7.19	90/120.4/90	547.8

Table 7: Pure silica zeolites: lattice parameters and cell volume.

Zeolite	a [Å]	b [Å]	c [Å]	$\alpha/\beta/\gamma$ [Deg]	Vol [Å^3]	Channel Dim.
(ITQ-29) LTA[21]	11.92	11.92	11.92	90	1693.2	3D
(ITQ-32) IHW[22]	13.70	24.02	18.20	90	6064.6	2D
(ITQ-3) ITE[23]	20.75	9.80	20.01	90	4071.1	2D (1D)
(SSZ-73) SAS[24]	14.10	14.10	10.18	90	2026.5	3D
Si-CHA[25]	13.67	13.67	14.76	90/120/90	2391.5	3D
(ITQ-12) ITW[26]	10.33	15.01	8.86	90/105.3/90	1353.9	2D(1D)

5 Structural properties of low density polymorphs computed with different FFs selected in the study.

5.1 Si-IHW (ITQ-32)

Table 8: *Si-IHW (ITQ-32): Lattice Parameters*

Potential	a [Å]	b [Å]	c [Å]	$\alpha = \beta = \gamma$ [Deg]	$Si - O$ [Å]	$Si - Si$ [Å]	$\angle Si - O - Si$	$\angle O - Si - O$
SLC	13.70	24.03	18.17	90	1.598	3.091	152	109.46
SS96	13.94	24.36	18.50	90	1.610	3.140	156	109.46
SS97	14.14	24.65	18.75	90	1.622	3.181	160	109.46
Gale	13.76	24.10	18.26	90	1.601	3.104	153	109.46
SC1	13.80	24.23	18.31	90	1.615	3.116	151	109.46
SC2	13.75	24.10	18.33	90	1.610	3.106	151	109.46
PMM08	13.82	24.29	18.26	90	1.628	3.120	148	109.46
JC	14.15	24.70	18.71	90	1.605	3.181	167	109.42
DSQFG	13.76	23.91	18.39	90	1.604	3.104	154	109.47
JA	14.04	23.17	13.10	90	-	-	-	-
AHCM	13.21	23.47	16.77	90	1.549	2.982	151	109.35
BKS	13.97	24.42	18.52	90	1.605	3.149	159	109.43
Vessal	14.21	24.66	18.69	90	1.608	3.187	166	109.42
PMM06	14.01	24.47	18.59	90	1.608	3.158	160	109.42
TTAM	14.30	24.99	18.95	90	1.641	3.222	160	109.42
BS	13.56	23.82	17.94	90	1.610	3.063	145	109.47
IZA	13.74	24.07	18.33	90	1.610	3.106	150.809	109.465
Exp[22]	13.70	24.02	18.20	90	1.595	-	-	109.478

5.2 Si-LTA (ITQ-29)

Table 9: *Si-LTA (ITQ-29): Lattice Parameters*

Potential	a=b=c [Å]	$\alpha = \beta = \gamma$ [Deg]	$Si - O$ [Å]	$Si - Si$ [Å]	$\angle Si - O - Si$	$\angle O - Si - O$
SLC	11.85	90	1.599	3.091	150	109.47
SS96	12.00	90	1.611	3.131	153	109.50
SS97	12.03	90	1.628	3.140	150	109.50
Gale	11.88	90	1.602	3.102	151	109.50
SC1	11.95	90	1.615	3.118	150	109.47
SC2	11.87	90	1.605	3.093	149	109.47
PMM08	12.02	90	1.628	3.137	150	109.47
JC	12.12	90	1.607	3.167	161	109.23
DSQFG	11.91	90	1.604	3.103	151	109.50
JA	12.05	90	1.611	3.148	156	109.30
AHCM	11.67	90	1.554	3.050	158	109.30
BKS	12.08	90	1.609	3.156	158	109.30
Vessal	12.11	90	1.610	3.172	161	109.20
PMM06	11.34	90	1.499	2.959	163	109.19
TTAM	12.36	90	1.645	3.230	159	109.31
BS	11.89	90	1.610	3.098	149	109.47
IZA	11.92	90	1.610	3.105	150	109.471
Exp [21]	11.87	90	1.600	-	153	109.40

5.3 Si-ITE (ITQ-3)

Table 10: *Si-ITE (ITQ-3): Lattice Parameters*

Potential	a [Å]	b [Å]	c [Å]	$\alpha = \beta = \gamma$ [Deg]	$Si-O$ [Å]	$Si-Si$ [Å]	$\angle Si-O-Si$	$\angle O-Si-O$
SLC	20.63	9.73	19.56	90	1.600	3.087	150	109.47
SS96	20.94	9.88	19.79	90	1.612	3.130	153	109.47
SS97	21.23	10.00	19.98	90	1.624	3.167	155	109.46
Gale	20.71	9.77	19.60	90	1.602	3.099	151	109.47
SC1	20.79	9.82	19.75	90	1.616	3.113	149	109.47
SC2	20.75	9.80	20.01	90	1.628	3.128	149	109.47
PMM08	20.65	9.80	19.87	90	1.629	3.110	147	109.47
JC	21.37	9.99	19.97	90	1.606	3.171	162	109.31
DSQFG	20.44	9.66	19.73	90	1.604	3.083	149	109.47
JA	19.93	9.71	19.74	90	1.608	3.069	147	109.39
AHCM	19.84	9.58	19.38	90	1.552	3.027	155	109.39
BKS	20.97	9.95	19.93	90	1.608	3.151	157	109.39
Vessal	21.27	10.01	19.93	90	1.609	3.175	161	109.30
PMM06	21.04	9.97	19.97	90	1.611	3.160	158	109.38
TTAM	21.49	10.18	20.38	90	1.644	3.225	158	109.38
BS	20.26	9.51	19.57	90	1.61	3.054	144	109.47
IZA	20.75	9.80	20.01	90	1.628	3.128	149	109.471
Exp [23]	20.62	9.72	19.62	90	1.60	-	-	109.4

5.4 Si-ITW (ITQ-12)

Table 11: *Si-ITW (ITQ-12): Lattice Parameters*

Potential	a [Å]	b [Å]	c [Å]	$\alpha = \gamma$ [Deg]	β [Deg]	$Si-O$ [Å]	$Si-Si$ [Å]	$\angle Si-O-Si$	$\angle O-Si-O$
SLC	10.30	15.05	8.86	90	105.24	1.599	3.089	151	109.47
SS96	10.41	15.27	8.99	90	105.20	1.612	3.131	154	109.46
SS97	10.50	15.47	9.10	90	105.13	1.624	3.167	156	109.45
Gale	10.32	15.11	8.89	90	105.16	1.602	3.101	152	109.47
SC1	10.40	15.17	8.94	90	105.28	1.615	3.116	151	109.47
SC2	10.45	15.03	8.95	90	105.64	1.610	3.099	150	109.47
PMM08	10.56	15.20	9.03	90	105.66	1.628	3.135	150	109.47
JC	10.37	15.58	9.08	90	104.87	1.606	3.167	162	109.31
DSQFG	10.40	14.99	8.94	90	105.65	1.604	3.090	150	109.47
JA	9.57	9.48	9.81	90	96.65	1.646	3.126	147	118.05
AHCM	10.18	15.48	7.92	90	105.63	1.551	3.019	157	109.39
BKS	10.40	15.55	8.90	90	104.78	1.607	3.150	159	109.39
Vessal	10.38	15.55	9.08	90	104.81	1.610	3.173	162	109.31
PMM06	10.45	15.54	8.94	90	104.97	1.610	3.159	159	109.38
TTAM	10.63	15.92	9.10	90	104.75	1.643	3.223	159	109.38
BS	10.48	14.90	8.90	90	105.63	1.61	3.081	148	109.47
IZA	10.45	15.03	8.95	90	105.64	1.610	3.10	150	109.471
Exp [27]	10.34	15.02	8.86	90	105.36	1.61	-	147	109.5

5.5 Si-SAS (SSZ-73)

Table 12: *Si-SAS (SSZ-73): Lattice Parameters*

Potential	a [Å]	c [Å]	$\alpha = \beta = \gamma$ [Deg]	$Si - O$ [Å]	$Si - Si$ [Å]	$\angle Si - O - Si$	$\angle O - Si - O$
SLC	14.03	10.21	90	1.599	3.089	150	109.476
SS96	14.23	10.34	90	1.611	3.131	153	109.466
SS97	14.42	10.43	90	1.624	3.167	154	109.5
Gale	14.08	10.24	90	1.602	3.100	151	109.474
SC1	14.16	10.31	90	1.615	3.117	150	109.476
SC2	14.07	10.30	90	1.605	3.104	151	109.470
PMM08	14.20	10.47	90	1.627	3.145	151	109.471
JC	14.47	10.38	90	1.607	3.167	161	109.359
DSQFG	14.17	10.26	90	1.604	3.112	152	109.471
JA	14.64	9.92	90	1.610	3.140	158	109.393
AHCM	13.98	9.87	90	1.553	3.044	158	109.391
BKS	14.43	10.28	90	1.608	3.152	157	109.396
Vessal	14.47	10.36	90	1.610	3.172	160	109.318
PMM06	13.56	9.668	90	1.499	2.962	163	109.381
TTAM	14.76	10.51	90	1.644	3.225	158	109.383
BS	14.12	10.32	90	1.61	3.113	150.55	109.45
IZA	14.35	10.40	90	1.627	3.152	151	109.471
Exp [24]	14.10	10.19	90	1.602	-	150	109.5

5.6 Si-CHA

Table 13: *Si-CHA: Lattice Parameters*

Potential	a [Å]	c [Å]	$\alpha = \beta$ [Deg]	γ [Deg]	$Si - O$ [Å]	$Si - Si$ [Å]	$\angle Si - O - Si$	$\angle O - Si - O$
SLC	13.55	14.58	90	120	1.602	3.077	148	109.47
SS96	13.71	14.84	90	120	1.613	3.119	150	109.47
SS97	13.85	15.04	90	120	1.625	3.154	152	109.46
Gale	13.60	14.61	90	120	1.605	3.089	149	109.47
SC1	13.67	14.77	90	120	1.619	3.109	147	109.47
SC2	13.62	14.71	90	120	1.605	3.091	149	109.47
PMM08	13.83	14.81	90	120	1.627	3.137	149	109.47
JC	13.87	15.06	90	120	1.608	3.159	158	109.34
DSQFG	13.61	14.81	90	120	1.604	3.095	149	109.47
JA	13.48	15.45	90	120	1.610	3.111	152	109.39
AHCM	13.22	6.19	90	120	1.665	3.094	141	105.31
BKS	13.85	14.82	90	120	1.609	3.140	153	109.39
Vessal	13.85	15.09	90	120	1.611	3.163	158	109.30
PMM06	12.98	14.09	90	120	1.499	2.953	160	109.36
TTAM	14.184	15.128	90	120	1.645	3.214	155	109.37
BS	13.66	14.76	90	120	1.61	3.099	148.53	109.47
IZA	13.67	14.77	90	120	1.610	3.103	149	109.471
Exp [25]	13.53	14.75	90	120	1.603	-	148	109.47

6 Mechanical and dielectric properties of α-Quartz

Table 14: α-Quartz Calculated and Experimental Mechanic Properties.

Potential	Bulk Modulus (GPa)	Elastic Constants [GPa]					
	K	C_{11}	C_{33}	C_{44}	C_{66}	C_{14}	C_{13}
SLC	44.41	94.66	112.57	49.68	39.94	-15.79	17.89
SS96	42.01	84.56	96.34	41.07	36.53	-13.70	23.94
SS97	45.35	75.89	105.64	38.14	26.10	-7.85	28.99
Gale	44.96	97.00	105.23	47.99	40.52	-16.28	18.60
SC1	43.37	91.80	113.21	48.57	38.26	-17.20	16.71
SC2	38.25	103.35	84.85	54.66	39.80	-16.97	3.90
PMM08	34.62	72.88	97.59	46.86	29.97	-13.34	11.77
JC	121.11	202.32	212.93	63.07	67.99	0.0001	86.27
DSQFG	0.000	31.71	28.13	32.92	13.62	-21.17	-22.56
JA	37.99	62.79	156.10	17.43	20.43	15.56	15.27
AHCM	43.54	69.27	176.32	36.30	23.04	1.658	24.65
BKS	40.10	90.55	107.07	50.27	41.22	-17.66	15.24
Vessal	199.16	318.10	301.87	78.61	99.49	-0.0001	154.46
PMM06	37.46	88.41	103.54	49.31	40.38	-18.33	11.03
TTAM	33.49	71.34	93.98	40.53	30.73	-13.76	12.73
BS	17.08	70.41	62.28	47.98	27.56	-17.04	-17.04
Exp [28]	38.98	86.83	105.98	58.26	39.87	-18.06	11.93

Table 15: α-Quartz Calculated and Experimental Dielectric Properties.

Potential	Static Dielectric Constant ϵ_{11}^0 - ϵ_{33}^0	High Frequency Dielectric Constant ϵ_{11}^∞ - ϵ_{33}^∞
SLC	4.58 - 4.88	2.07 - 2.09
SS96	4.07 - 4.42	1.75 - 1.76
SS97	4.47 - 4.65	1.84 - 1.86
Gale	4.81 - 5.29	1.98 - 1.99
SC1	3.32 - 3.53	1.91 - 1.93
SC2	4.14 - 4.26	3.09 - 3.21
PMM08	2.78 - 2.84	1.423 - 1.425
JC	3.90 - 4.07	——-
DSQFG	1.00 - 1.00	——-
JA	2.33 - 2.34	——-
AHCM	2.31 - 2.36	——-
BKS	1.95 - 1.99	——-
Vessal	3.68 - 3.83	——-
PMM06	2.25 - 2.32	——-
TTAM	2.11 - 2.17	——-
BS	——-	——-
Exp[29]	4.51 - 4.60	2.4 - 2.4

7 8-ring diameters obtained from MD simulations for the low density silica polymorphs.

7.1 Si-IHW (ITQ-32)

Table 16: 8-ring diameters for Si-IHW, computed as the radial distribution functions of the O-O inter-atomic distances along the MD simulations performed at 300 K, within the NVE ensemble.

Potential	D1 [Å]	D2 [Å]
BKS	3.90±0.18	4.30±0.20
PMM06	3.93±0.18	4.27±0.20
TTAM	4.04±0.21	4.49±0.22
BS	3.38±0.22	4.35±0.25
IZA	3.5	4.3

Figure 2: Si-IHW rings

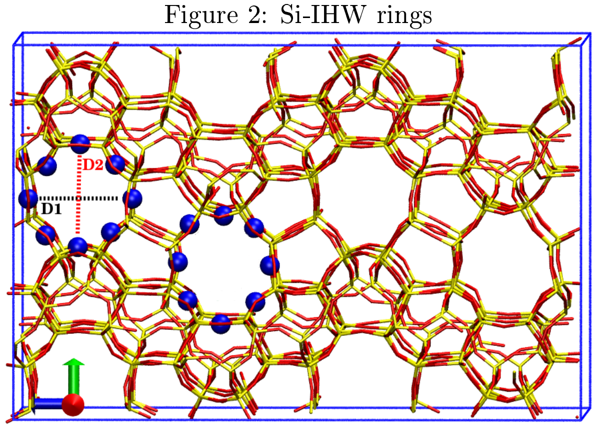
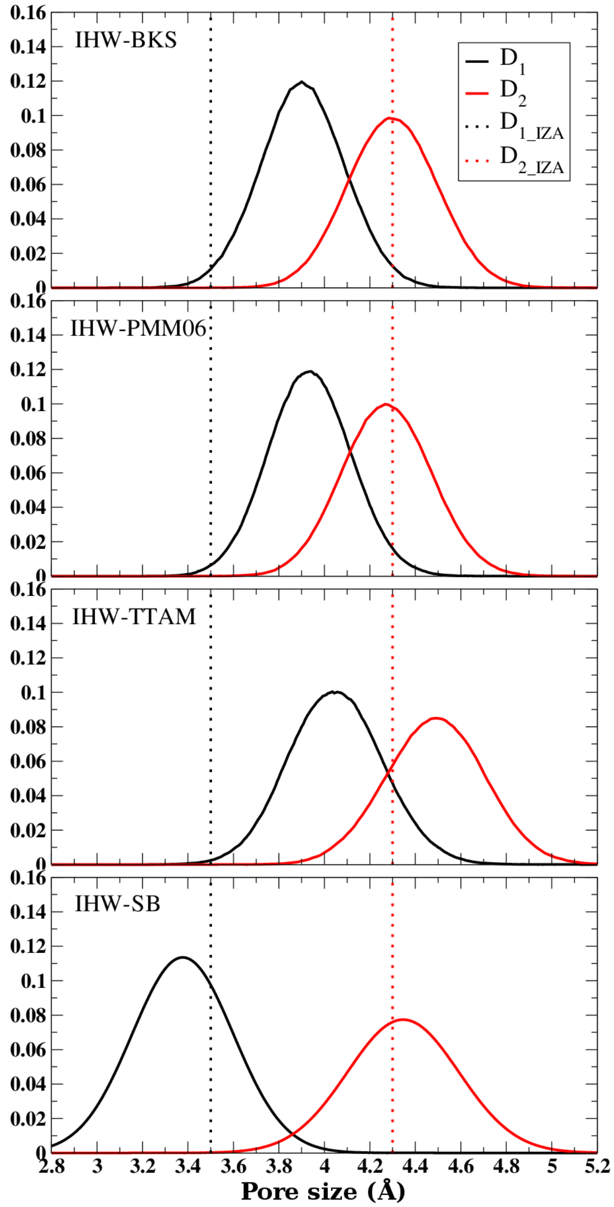


Figure 3: 8-ring diameters computed as the radial distribution function of the O-O distance, computed via MD simulations for Si-IHW.



7.2 Si-LTA (ITQ-29)

Table 17: Window Diameters for Si-LTA, computed as the radial distribution functions of the O-O inter-atomic distances along the MD simulations performed at 300 K, within the NVE ensemble.

Potential	D1 [Å]
BKS	4.10±0.17
PMM06	4.09±0.15
TTAM	4.24±0.19
BS	4.13±0.17
IZA	4.2

Figure 4: Si-LTA rings

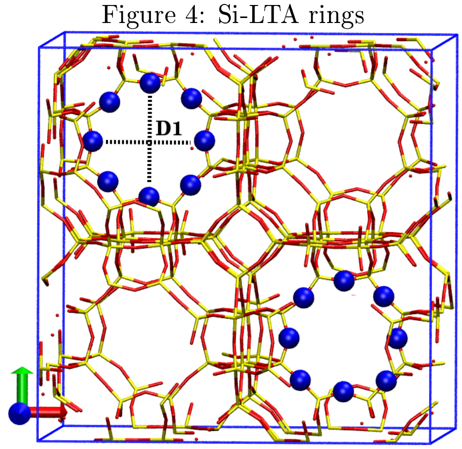


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Figure 5: 8-ring diameters computed as the radial distribution function of the O-O distance, computed via MD simulations for Si-LTA.

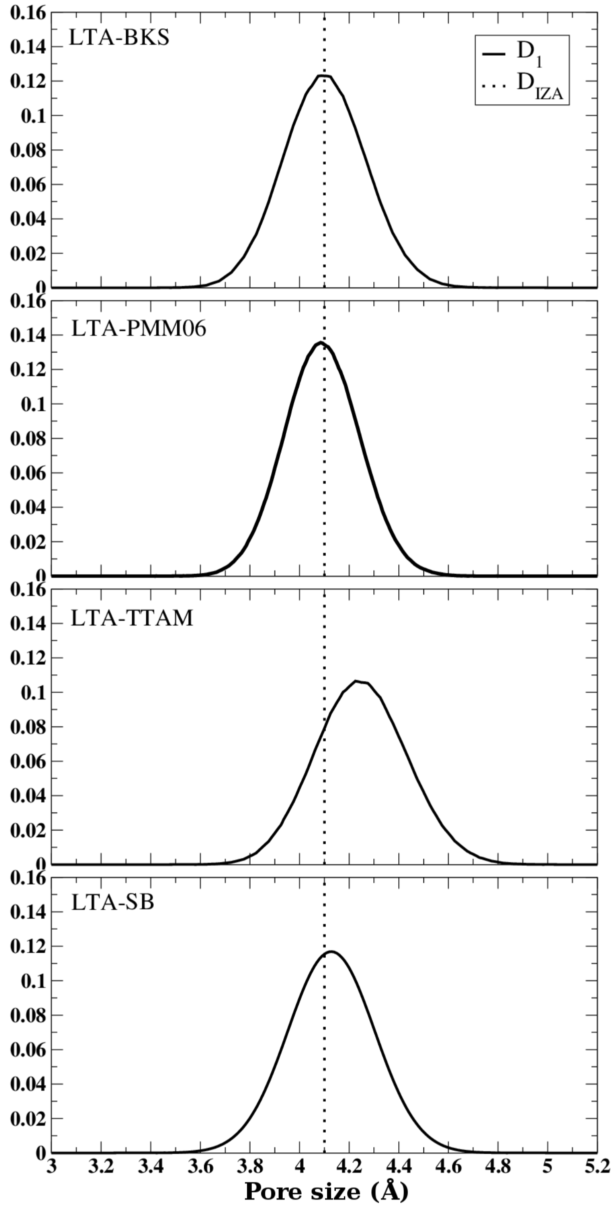
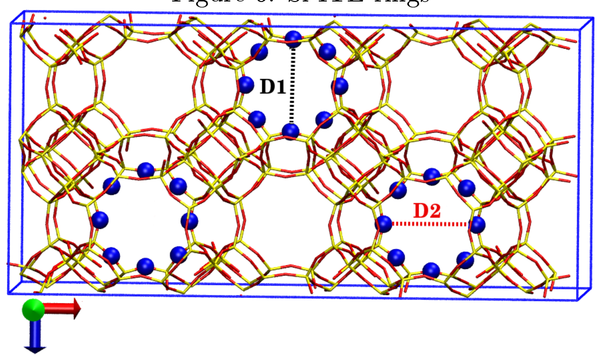


Figure 6: Si-ITE rings

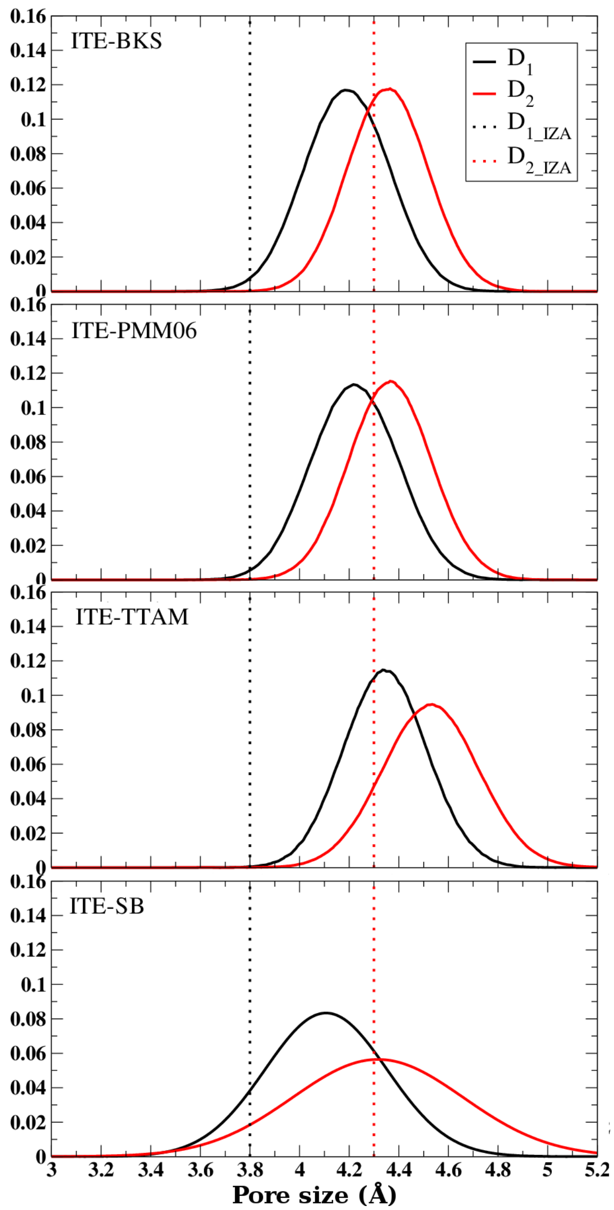


7.3 Si-ITE (ITQ-3)

Table 18: Window Diameters for Si-ITE, computed as the radial distribution functions of the O-O inter-atomic distances along the MD simulations performed at 300 K, within the NVE ensemble.

Potential	D1 [Å]	D2 [Å]
BKS	4.19±0.17	4.35±0.16
PMM06	4.22±0.18	4.36±0.17
TTAM	4.34±0.17	4.53±0.19
BS	4.10±0.24	4.32±0.35
IZA	3.8	4.3

Figure 7: 8-ring diameters computed as the radial distribution function of the O-O distance, computed via MD simulations for Si-ITE.



7.4 Si-ITW (ITQ-12)

Table 19: Window Diameters for Si-ITW, computed as the radial distribution functions of the O-O inter-atomic distances along the MD simulations performed at 300 K, within the NVE ensemble.

Potential	**D1 [Å]**	**D2 [Å]**
BKS	3.78±0.23	4.26±0.23
PMM06	3.83±0.19	4.29±0.20
TTAM	4.08±0.22	4.76±0.22
BS	4.08±0.20	4.12±0.24
IZA	3.9	4.2

Figure 8: Si-ITW rings

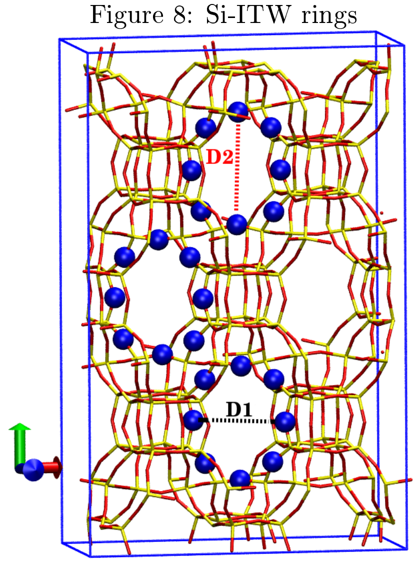
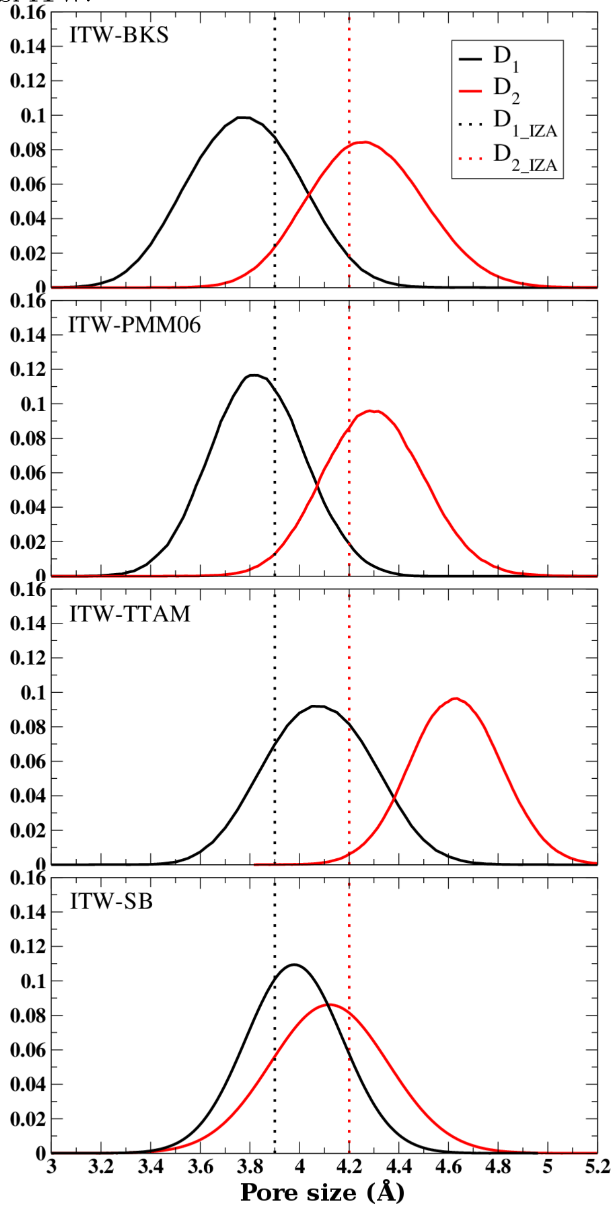


Figure 9: 8-ring diameters computed as the radial distribution function of the O-O distance, computed via MD simulations for Si-ITW.



7.5 Si-SAS (SSZ-73)

Table 20: Window Diameters for Si-SAS, computed as the radial distribution functions of the O-O inter-atomic distances along the MD simulations performed at 300 K, within the NVE ensemble.

Potential	**D1 [Å]**
BKS	4.23±0.16
PMM06	4.22±0.16
TTAM	4.40±0.17
BS	4.19±0.17
IZA	4.2

Figure 10: Si-SAS rings

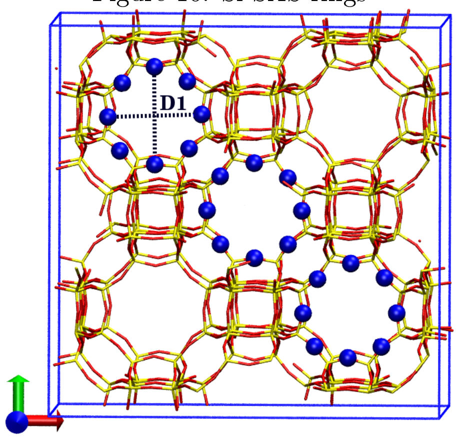
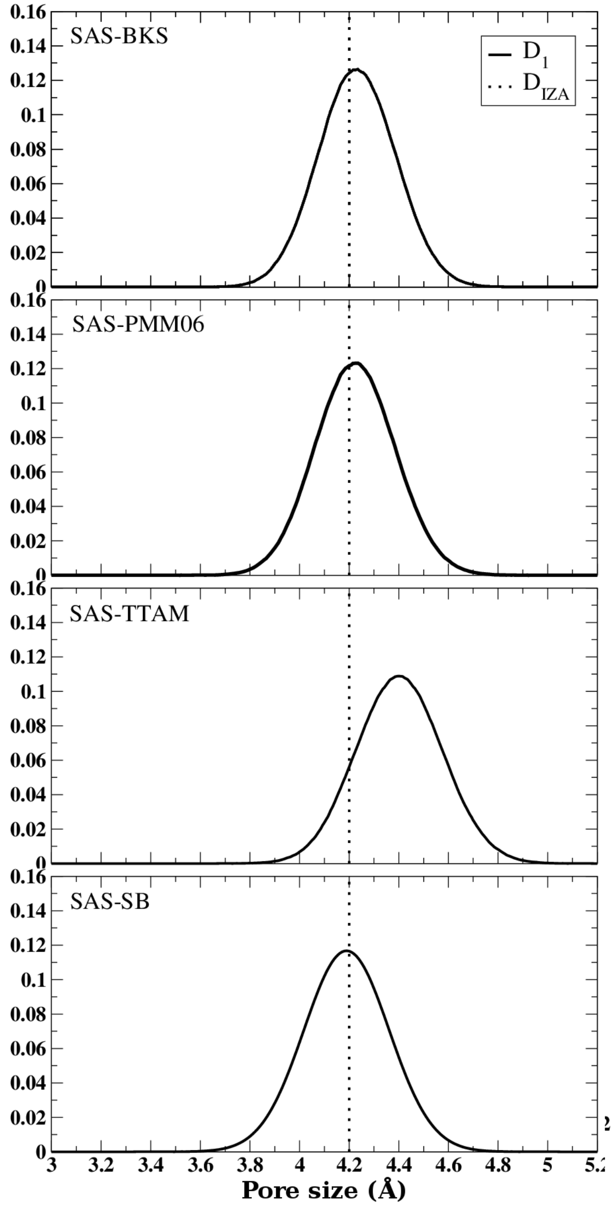


Figure 11: 8-ring diameters computed as the radial distribution function of the O-O distance, computed via MD simulations for Si-SAS.



7.6 Si-CHA

Table 21: Window Diameters for Si-CHA, computed as the radial distribution functions of the O-O inter-atomic distances along the MD simulations performed at 300 K, within the NVE ensemble.

Potential	**D1 [Å]**
BKS	3.77±0.20
PMM06	3.89±0.17
TTAM	3.92±0.21
BS	3.65±0.18
IZA	3.8

Figure 12: Si-CHA rings

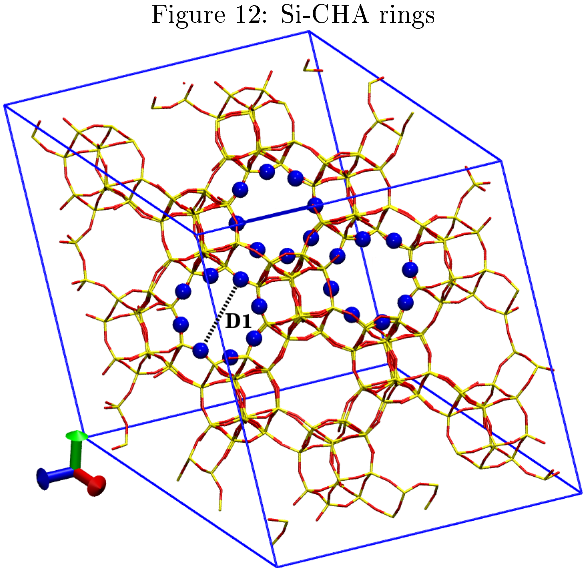
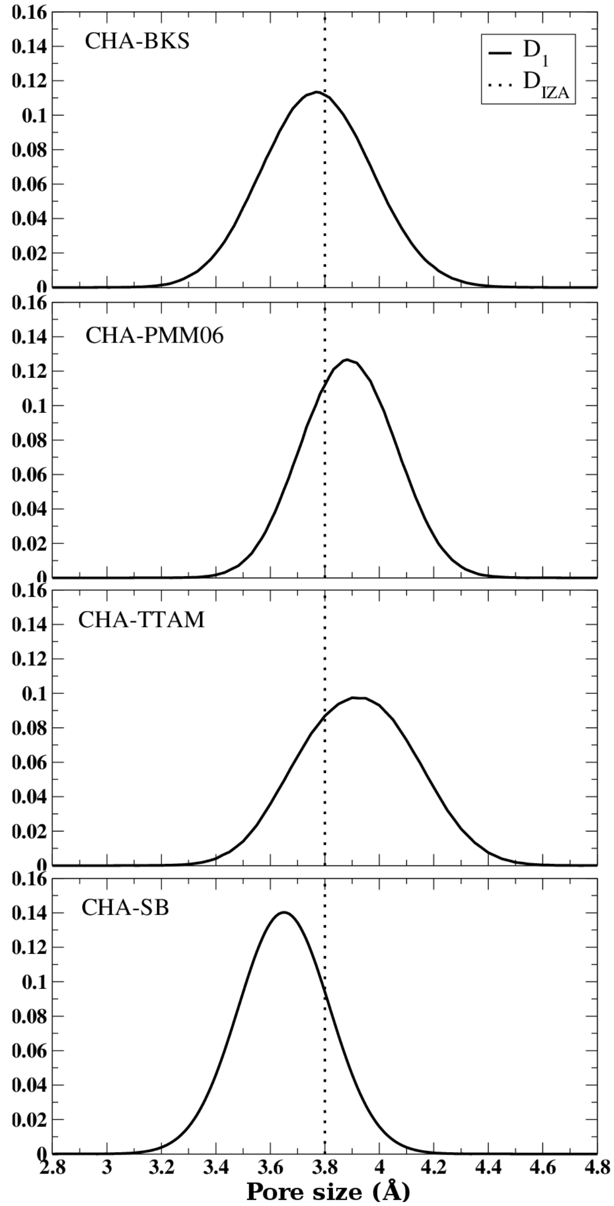


Figure 13: 8-ring diameters computed as the radial distribution function of the O-O distance, computed via MD simulations for Si-CHA.



8 Relative errors computed for the structural parameters.

Figure 14: Relative error (%) computed for structural parameters of the pure silica polymorphs, α-quartz, β-quartz and coesite, calculated with the selected FFs.

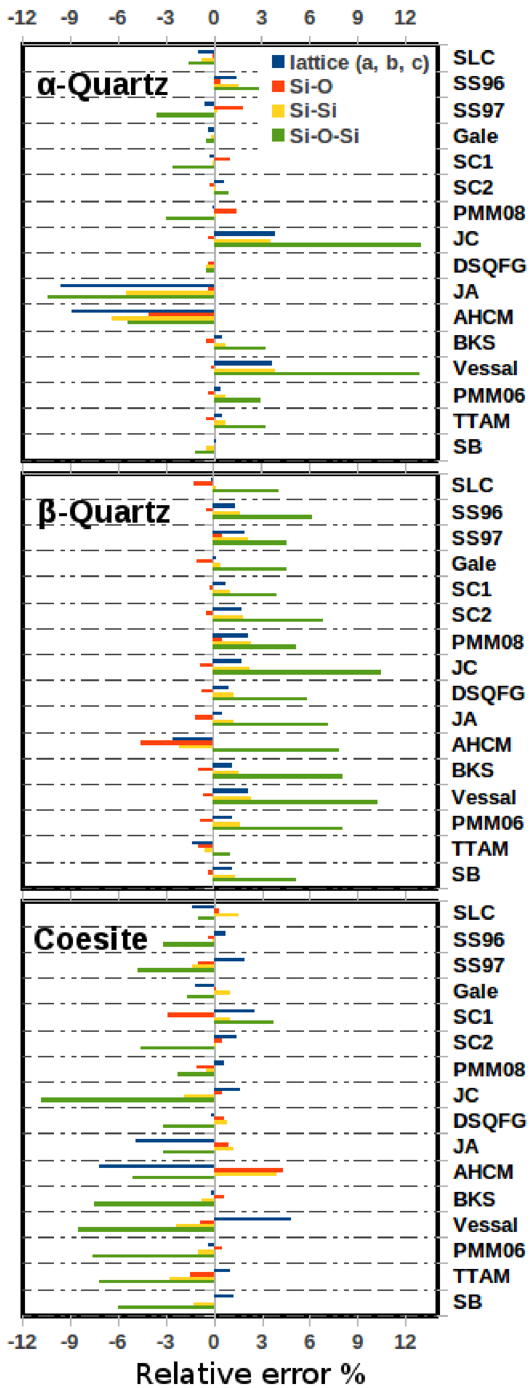
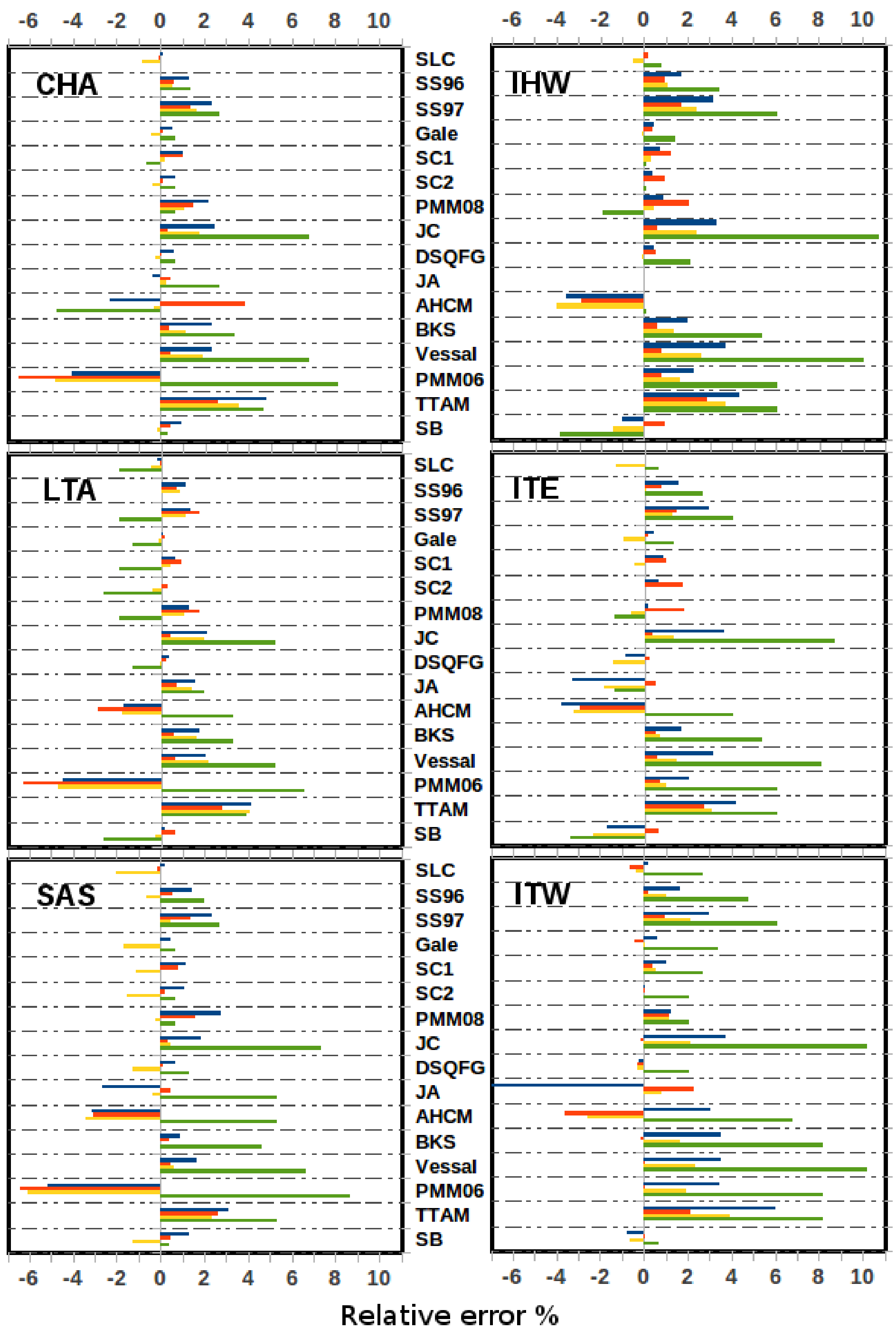


Figure 15: Relative error (%) computed for structural parameters of pure silica zeolites CHA, LTA, SAS, IHW, ITE and ITW, calculated with the selected FFs.



9 Pore volume of selected low density silica polymorphs.

As additional test, in order to compare the performance of the four selected rigid ions FFs, the pore volume of the minimized structures were computed and compared with the values estimeted by nitrogen or argon adsorption experiments, where available. The pore volumes were estimated with the PLATON code [30] employing the Lennard-Jones sigma value of a nitrogen molecule (3.68Å) and the van der Waals diameter of the Argon atom (3.84 Å) according to previous works [31].

Table 22: Experimental and calculated Pore Volumes (cm^3/g).

	IZA(Exp.)		BKS		PMM06		TTAM		BS	
	N_2	Ar	N_2	Ar	N_2	Ar	N_2	Ar	N_2	Ar
Si-IHW	0.13 (0.16[22], 0.17[32])	0.12	0.14	0.14	0.14	0.14	0.16	0.16	0.11	0.10
Si-LTA	0.31 (0.32[33])	0.32 (0.24[**21**])	0.35	0.33	0.35	0.34	0.37	0.37	0.32	0.32
Si-ITE	0.23 (0.23[34])	0.23	0.24	0.24	0.25	0.24	0.27	0.27	0.20	0.20
Si-ITW	0.13	0.10 (0.15[35])	0.13	0.08	0.14	0.08	0.15	0.15	0.13	0.07
Si-SAS	0.23 (0.25[**21**])	0.23	0.26	0.26	0.26	0.26	0.29	0.28	0.23	0.24
Si-CHA	0.26 (0.30[34])	0.26	0.28	0.27	0.29	0.27	0.32	0.31	0.26	0.26

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