Table S-I. Lattice constants for silica polymorphs from the experiment^{a-f} and NPT simulations using MS-Q.

	ρ g/cc	A Å	B Å	C Å	α deg	β deg	γ deg
α-quartz [Hexagonal($P3_121$)]							
Exp. (RT)[a]	2.646	4.9160	4.9160	5.4054	90.00	90.00	120.00
This Work (300 K)	2.579	4.9772	4.9820	5.4268	90.05	90.02	120.01
β-quartz [Hexagonal($P6_222$)]							
Exp. (863 K)[b]	2.534	5.0100	5.0100	5.4700	90.00	90.00	120.00
This Work (863 K)	2.549	5.0143	5.0096	5.4353	89.97	90.02	120.00
Stishovite [Tetragonal($P4_2/mnm$)]							
Exp. (RT)[c]	4.281	4.1801	4.1801	2.6678	90.00	90.00	90.00
This Work (300 K)	4.254	4.2388	4.2376	2.6154	89.99	90.01	90.08
β-tridymite [Hexagonal($P6_3/mmc$)]							
Exp. (733 K)[d]	2.183	5.0300	5.0300	8.2200	90.00	90.00	120.00
This Work (733 K)	2.273	5.0112	5.0091	8.1391	89.89	90.43	119.83
α-cristobalite [Tetragonal($P4_12_12$)]							
Exp. (303 K)[e]	2.334	4.9570	4.9570	6.8903	90.00	90.00	90.00
This Work (303 K)	2.550	4.9406	4.9266	6.4706	90.01	89.99	89.95
β-cristobalite [Cubic(Fd3m)]							
Exp. (573 K)[e]	2.205	7.1600	7.1600	7.1600	90.00	90.00	90.00
This Work (573 K)	2.435	6.9102	7.0276	6.7901	89.98	89.94	90.00
Keatite [Tetragonal ($P4_32_12$)]							
Exp. (RT)[b]	2.499	7.4600	7.4600	8.6100	90.00	90.00	90.00
This Work (300 K)	2.550	7.5366	7.5559	8.2529	89.98	89.96	90.02
Coesite [Pseudo-hexagonal(C2/c)]							
Exp. (RT)[f]	2.921	7.1356	12.3692	7.1736	90.00	120.34	90.00
This Work (300 K)	2.813	7.2077	12.5370	7.2646	89.97	120.13	90.01

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