Support information

New insight into the plastic deformation mechanisms during SiO_2 phase transition process

Zhenlun Wei[a], Yubiao Li[a,b]*, Peiyue Li[c,d], Li Pan[d], Wanqing Li[a], Xianglin Hu[a], Yunxiang Gu[a]

[a] *School of Resources and Environmental Engineering, Wuhan University of Technology, Wuhan 430070, Hubei, China;*

[b] *Key Laboratory of Green Utilization of Critical Non-metallic Mineral Resources, Ministry of Education, Wuhan 430070, Hubei, China;*

[c] *(Anhui) National Innovation Center for Advanced Glass Materials, Bengbu, Anhui, 233018, PR China;*

[d] *CNBM Research Institute for Advanced Glass Materials Group Co., Ltd, Bengbu, 233018, PR China.*

*Corresponding author. Email: yubiao.li@whut.edu.cn (Y. Li)

Address: 122, Luoshi Road, Hongshan District, Wuhan, Hubei, China, 430070

This supporting information contains 15 pages, 3 figures and 5 tables.

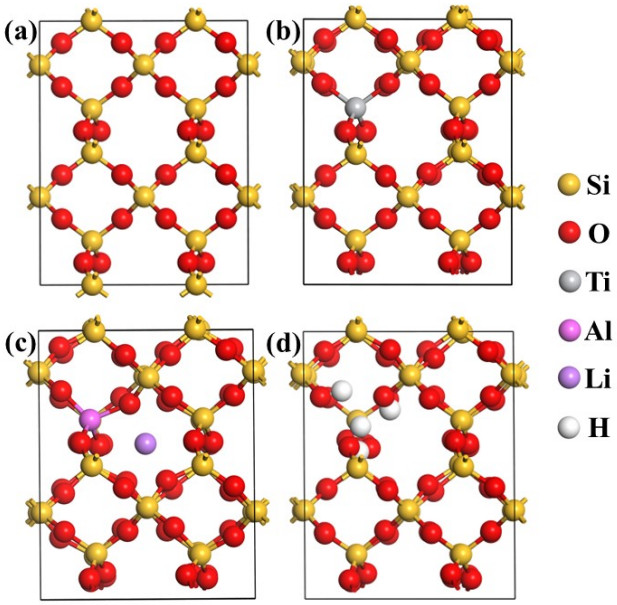

Fig.S1 Structures of optimized and Ti^{4+}, Al^{3+}/Li^{+} and $4H^{+}$ substituted 2×2×2 β-quartz supercells: (a) $Si_{24}O_{48}$; (b) $Si_{23}TiO_{48}$; (c) $Si_{23}AlLiO_{48}$; (d) $Si_{23}H_4O_{48}$

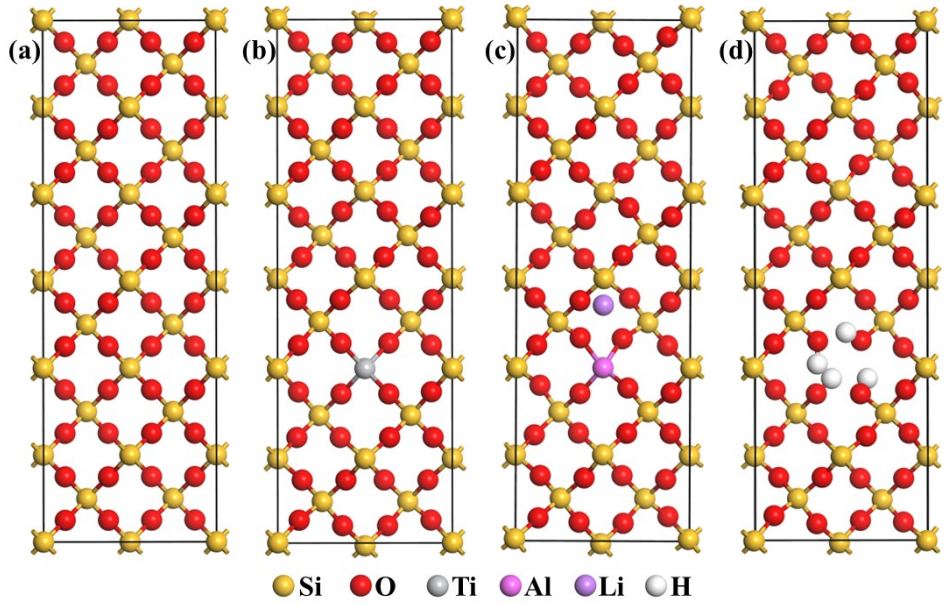

Fig.S2 Structures of optimized and Ti^{4+}, Al^{3+}/Li^{+} and $4H^{+}$ substituted 3×1×1 β-cristobalite supercells: (a) $Si_{24}O_{48}$; (b) $Si_{23}TiO_{48}$; (c) $Si_{23}AlLiO_{48}$; (d) $Si_{23}H_4O_{48}$

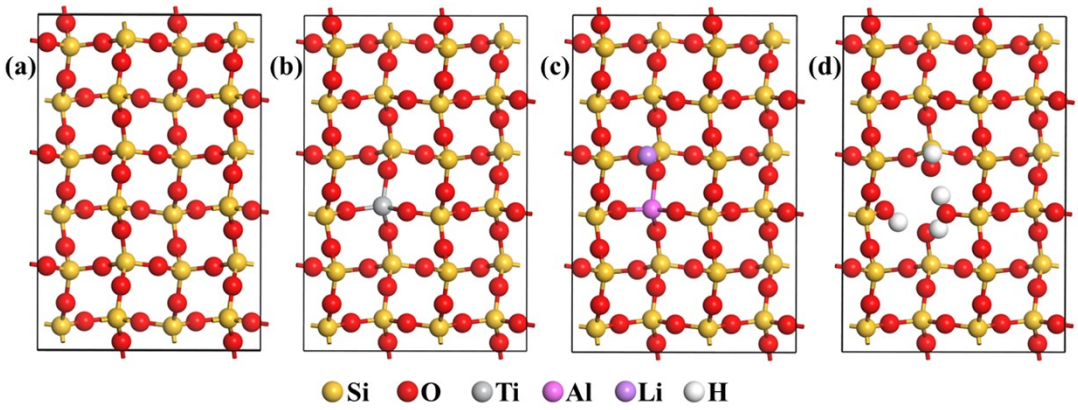

Fig.S3 Structures of optimized and Ti^{4+}, Al^{3+}/Li^{+} and $4H^{+}$ substituted 3×2×1 α-cristobalite supercells: (a) $Si_{24}O_{48}$; (b) $Si_{23}TiO_{48}$; (c) $Si_{23}AlLiO_{48}$; (d) $Si_{23}H_4O_{48}$

Table S1 The xyz coordinates for transition state structures in original SiO_2 phases, TS1 was the transition state between α-quartz and β-quartz, TS2 was the transition state between β-quartz and β-cristobalite, TS3 was the transition state between β-cristobalite and α-cristobalite.

Atom number	TS1			TS2			TS3		
	x	y	z	x	y	z	x	y	z
Si1	0.250000	0.000000	-0.000041	0.000000	0.000000	0.000000	0.099836	0.149763	0.000001
Si2	0.000000	0.250000	0.333374	0.000000	0.500000	0.500000	0.233498	0.350237	0.500001
Si3	0.250000	0.250000	0.166667	0.166673	0.000000	0.500000	0.066831	0.399763	0.249999
Si4	0.750000	0.000000	-0.000041	0.166673	0.500000	0.000000	0.266502	0.100237	0.749999
Si5	0.500000	0.250000	0.333374	0.250000	0.250000	0.750000	0.433169	0.149763	0.000001
Si6	0.750000	0.250000	0.166667	0.083327	0.250000	0.250000	0.566831	0.350237	0.500001
Si7	0.250000	0.500000	-0.000041	0.083327	0.750000	0.750000	0.400165	0.399763	0.249999
Si8	0.000000	0.750000	0.333374	0.250000	0.750000	0.250000	0.599835	0.100237	0.749999
Si9	0.250000	0.750000	0.166667	0.333327	0.000000	0.000000	0.766502	0.149763	0.000001
Si10	0.750000	0.500000	-0.000041	0.333327	0.500000	0.500000	0.900164	0.350237	0.500001
Si11	0.500000	0.750000	0.333374	0.500000	0.000000	0.500000	0.733498	0.399763	0.249999
Si12	0.750000	0.750000	0.166667	0.500000	0.500000	0.000000	0.933169	0.100237	0.749999
Si13	0.250000	0.000000	0.499959	0.583327	0.250000	0.750000	0.099836	0.649763	0.000001
Si14	0.000000	0.250000	0.833374	0.416673	0.250000	0.250000	0.233498	0.850237	0.500001
Si15	0.250000	0.250000	0.666667	0.416673	0.750000	0.750000	0.066831	0.899763	0.249999
Si16	0.750000	0.000000	0.499959	0.583327	0.750000	0.250000	0.266502	0.600237	0.749999
Si17	0.500000	0.250000	0.833374	0.666673	0.000000	0.000000	0.433169	0.649763	0.000001
Si18	0.750000	0.250000	0.666667	0.666673	0.500000	0.500000	0.566831	0.850237	0.500001
Si19	0.250000	0.500000	0.499959	0.833327	0.000000	0.500000	0.400165	0.899763	0.249999
Si20	0.000000	0.750000	0.833374	0.833327	0.500000	0.000000	0.599835	0.600237	0.749999
Si21	0.250000	0.750000	0.666667	0.916673	0.250000	0.750000	0.766502	0.649763	0.000001
Si22	0.750000	0.500000	0.499959	0.750000	0.250000	0.250000	0.900164	0.850237	0.500001
Si23	0.500000	0.750000	0.833374	0.750000	0.750000	0.750000	0.733498	0.899763	0.249999
Si24	0.750000	0.750000	0.666667	0.916673	0.750000	0.250000	0.933169	0.600237	0.749999
O1	0.204849	0.102237	0.083323	0.041695	0.124980	0.124980	0.080322	0.051959	0.178422
O2	0.397702	0.102298	0.416667	0.041695	0.624980	0.624980	0.253012	0.448041	0.678422
O3	0.397763	0.295151	0.250010	0.208305	0.125020	0.625020	0.132020	0.370489	0.428391
O4	0.295151	0.397763	0.083323	0.208305	0.625020	0.125020	0.201313	0.129511	0.928391
O5	0.102298	0.397702	0.416667	0.291695	0.374980	0.625020	0.086345	0.301959	0.071578
O6	0.102237	0.204849	0.250010	0.291695	0.874980	0.125020	0.246988	0.198041	0.571578
O7	0.704849	0.102237	0.083323	0.125000	0.875000	0.625000	0.034647	0.120489	0.821609
O8	0.897702	0.102298	0.416667	0.125000	0.625000	0.875000	0.298687	0.379511	0.321609
O9	0.897763	0.295151	0.250010	0.125000	0.125000	0.375000	0.413655	0.051959	0.178422
O10	0.795151	0.397763	0.083323	0.291695	0.625020	0.374980	0.586345	0.448041	0.678422

O11	0.602298	0.397702	0.416667	0.208305	0.874980	0.374980	0.465353	0.370489	0.428391
O12	0.602237	0.204849	0.250010	0.208305	0.374980	0.874980	0.534647	0.129511	0.928391
O13	0.204849	0.602237	0.083323	0.041695	0.875020	0.875020	0.419678	0.301959	0.071578
O14	0.397702	0.602298	0.416667	0.291695	0.125020	0.874980	0.580322	0.198041	0.571578
O15	0.397763	0.795151	0.250010	0.125000	0.375000	0.125000	0.367980	0.120489	0.821609
O16	0.295151	0.897763	0.083323	0.041695	0.375020	0.375020	0.632020	0.379511	0.321609
O17	0.102298	0.897702	0.416667	0.375000	0.125000	0.125000	0.746988	0.051959	0.178422
O18	0.102237	0.704849	0.250010	0.375000	0.625000	0.625000	0.919678	0.448041	0.678422
O19	0.704849	0.602237	0.083323	0.541695	0.124980	0.624980	0.798687	0.370489	0.428391
O20	0.897702	0.602298	0.416667	0.541695	0.624980	0.124980	0.867980	0.129511	0.928391
O21	0.897763	0.795151	0.250010	0.625000	0.375000	0.625000	0.753012	0.301959	0.071578
O22	0.795151	0.897763	0.083323	0.625000	0.875000	0.125000	0.913655	0.198041	0.571578
O23	0.602298	0.897702	0.416667	0.458305	0.875020	0.624980	0.701313	0.120489	0.821609
O24	0.602237	0.704849	0.250010	0.458305	0.624980	0.875020	0.965353	0.379511	0.321609
O25	0.204849	0.102237	0.583323	0.458305	0.124980	0.375020	0.080322	0.551959	0.178422
O26	0.397702	0.102298	0.916667	0.625000	0.625000	0.375000	0.253012	0.948041	0.678422
O27	0.397763	0.295151	0.750010	0.541695	0.875020	0.375020	0.132020	0.870489	0.428391
O28	0.295151	0.397763	0.583323	0.541695	0.375020	0.875020	0.201313	0.629511	0.928391
O29	0.102298	0.397702	0.916667	0.375000	0.875000	0.875000	0.086345	0.801959	0.071578
O30	0.102237	0.204849	0.750010	0.625000	0.125000	0.875000	0.246988	0.698041	0.571578
O31	0.704849	0.102237	0.583323	0.458305	0.375020	0.124980	0.034647	0.620489	0.821609
O32	0.897702	0.102298	0.916667	0.375000	0.375000	0.375000	0.298687	0.879511	0.321609
O33	0.897763	0.295151	0.750010	0.708305	0.125020	0.125020	0.413655	0.551959	0.178422
O34	0.795151	0.397763	0.583323	0.708305	0.625020	0.625020	0.586345	0.948041	0.678422
O35	0.602298	0.397702	0.916667	0.875000	0.125000	0.625000	0.465353	0.870489	0.428391
O36	0.602237	0.204849	0.750010	0.875000	0.625000	0.125000	0.534647	0.629511	0.928391
O37	0.204849	0.602237	0.583323	0.958305	0.375020	0.624980	0.419678	0.801959	0.071578
O38	0.397702	0.602298	0.916667	0.958305	0.875020	0.124980	0.580322	0.698041	0.571578
O39	0.397763	0.795151	0.750010	0.791695	0.874980	0.625020	0.367980	0.620489	0.821609
O40	0.295151	0.897763	0.583323	0.791695	0.625020	0.874980	0.632020	0.879511	0.321609
O41	0.102298	0.897702	0.916667	0.791695	0.125020	0.374980	0.746988	0.551959	0.178422
O42	0.102237	0.704849	0.750010	0.958305	0.624980	0.375020	0.919678	0.948041	0.678422
O43	0.704849	0.602237	0.583323	0.875000	0.875000	0.375000	0.798687	0.870489	0.428391
O44	0.897702	0.602298	0.916667	0.875000	0.375000	0.875000	0.867980	0.629511	0.928391
O45	0.897763	0.795151	0.750010	0.708305	0.874980	0.874980	0.753012	0.801959	0.071578
O46	0.795151	0.897763	0.583323	0.958305	0.124980	0.875020	0.913655	0.698041	0.571578
O47	0.602298	0.897702	0.916667	0.791695	0.374980	0.125020	0.701313	0.620489	0.821609
O48	0.602237	0.704849	0.750010	0.708305	0.374980	0.374980	0.965353	0.879511	0.321609

Table S2 The xyz coordinates for transition state structures in Ti^{4+} substituted SiO_2 phases, Ti-S-TS1 was the transition state between Ti^{4+} substituted α-quartz and Ti^{4+} substituted β-quartz, Ti-S-TS2 was the transition state between Ti^{4+} substituted β-quartz and Ti^{4+} substituted β-cristobalite, Ti-S-TS3 was the transition state between Ti^{4+} substituted β-cristobalite and Ti^{4+} substituted α-cristobalite.

Atom number	Ti-S-TS1			Ti-S-TS2			Ti-S-TS3		
	x	y	z	x	y	z	x	y	z
Si1	0.249951	-0.000117	0.000328	-0.000004	0.000000	0.000000	0.095954	0.144015	0.000007
Si2	-0.000117	0.249951	0.333005	-0.000005	0.500000	0.500000	0.237382	0.355993	0.499929
Si3	0.250000	0.250000	0.166667	0.166655	0.000000	0.500000	0.070717	0.394013	0.250002
Si4	0.749736	-0.000279	0.000460	0.166655	0.500000	0.000000	0.262610	0.105985	0.749986
Si5	0.500117	0.250049	0.333005	0.249306	0.247938	0.752062	0.429278	0.143997	0.000004
Si6	0.750000	0.250000	0.166691	0.083333	0.250000	0.250000	0.403765	0.394078	0.249848
Si7	0.250049	0.500117	0.000328	0.083333	0.750000	0.750000	0.596000	0.105571	0.750162
Si8	-0.000279	0.749736	0.332874	0.249306	0.752062	0.247938	0.762631	0.144034	0.000017
Si9	0.250000	0.750000	0.166643	0.333339	0.000000	0.000000	0.904054	0.355981	0.500017
Si10	0.750264	0.500279	0.000460	0.500006	0.000000	0.500000	0.737559	0.394092	0.249461
Si11	0.500279	0.750264	0.332874	0.500006	0.500000	0.000000	0.929288	0.105978	0.750005
Si12	0.750000	0.750000	0.166667	0.583345	0.250000	0.750000	0.095954	0.644011	0.000005
Si13	0.251684	-0.007603	0.494756	0.417355	0.247936	0.247936	0.237374	0.855981	0.500004
Si14	-0.007603	0.251684	0.838577	0.417355	0.752064	0.752064	0.070708	0.894012	0.249995
Si15	0.749929	-0.000087	0.500232	0.583345	0.750000	0.250000	0.262617	0.605979	0.749994
Si16	0.507603	0.248316	0.838577	0.666665	0.000000	0.000000	0.429305	0.644026	-0.000011
Si17	0.750000	0.250000	0.666589	0.666666	0.500000	0.500000	0.570714	0.856022	0.500058
Si18	0.248316	0.507603	0.494756	0.833339	0.000000	0.500000	0.404041	0.893995	0.249998
Si19	-0.000087	0.749929	0.833102	0.833339	0.500000	0.000000	0.596007	0.606281	0.750530
Si20	0.250000	0.750000	0.666744	0.916659	0.250003	0.749997	0.762614	0.644005	0.000002
Si21	0.750071	0.500087	0.500232	0.750003	0.250003	0.250003	0.904041	0.855981	0.500003
Si22	0.500087	0.750071	0.833102	0.750003	0.749997	0.749997	0.737378	0.894000	0.249988
Si23	0.750000	0.750000	0.666667	0.916659	0.749997	0.250003	0.929286	0.605990	0.750009
Ti1	0.250000	0.250000	0.666667	0.333333	0.500000	0.500000	0.570847	0.356182	0.500057
O1	0.211795	0.105668	0.083430	0.041702	0.124947	0.124947	0.082587	0.039812	0.167947
O2	0.395166	0.106425	0.416089	0.041737	0.624949	0.624949	0.250746	0.460189	0.667962
O3	0.394332	0.288205	0.249903	0.208246	0.124862	0.624963	0.140244	0.373912	0.417711
O4	0.288205	0.394332	0.083430	0.208246	0.624963	0.124862	0.193091	0.126082	0.917710
O5	0.104834	0.393575	0.416089	0.288939	0.366547	0.633453	0.084077	0.289811	0.082051
O6	0.105668	0.211795	0.249903	0.291727	0.875111	0.124889	0.249260	0.210172	0.582068
O7	0.711628	0.105625	0.083418	0.125000	0.874975	0.625009	0.026416	0.123911	0.832285
O8	0.894183	0.106091	0.416739	0.125000	0.625009	0.874975	0.306810	0.376072	0.332275

O9	0.894310	0.288204	0.249936	0.125000	0.125025	0.374991	0.415926	0.039822	0.167946
O10	0.788372	0.394375	0.083418	0.288939	0.633453	0.366547	0.584911	0.466391	0.677449
O11	0.605817	0.393909	0.416739	0.208246	0.875138	0.375037	0.467855	0.375000	0.412541
O12	0.605690	0.211796	0.249936	0.208246	0.375037	0.875138	0.526411	0.126115	0.917741
O13	0.211796	0.605690	0.083397	0.041702	0.875053	0.875053	0.417435	0.289798	0.082025
O14	0.395156	0.607903	0.415049	0.291727	0.124889	0.875111	0.583300	0.201581	0.587187
O15	0.394375	0.788372	0.249915	0.125000	0.374991	0.125025	0.359764	0.123915	0.832293
O16	0.288204	0.894310	0.083397	0.041737	0.375051	0.375051	0.644389	0.377345	0.322735
O17	0.104844	0.892097	0.415049	0.374973	0.124840	0.124840	0.749248	0.039811	0.167954
O18	0.105625	0.711628	0.249915	0.377764	0.633397	0.633397	0.917403	0.460178	0.667938
O19	0.711798	0.605632	0.083349	0.541699	0.124974	0.624958	0.806893	0.373908	0.417732
O20	0.894067	0.605985	0.416578	0.541699	0.624958	0.124974	0.859752	0.126079	0.917706
O21	0.894368	0.788202	0.249984	0.624962	0.375000	0.625000	0.750779	0.289732	0.081970
O22	0.788202	0.894368	0.083349	0.624997	0.875002	0.124998	0.915916	0.210188	0.582046
O23	0.605933	0.894015	0.416578	0.458354	0.875239	0.624861	0.693095	0.123932	0.832312
O24	0.605632	0.711798	0.249984	0.458354	0.624861	0.875239	0.973569	0.376083	0.332296
O25	0.203949	0.090798	0.575865	0.458354	0.124761	0.375139	0.082585	0.539814	0.167946
O26	0.393575	0.104834	0.917245	0.624962	0.625000	0.375000	0.250749	0.960184	0.667950
O27	0.409202	0.296051	0.757468	0.541699	0.875026	0.375042	0.140249	0.873911	0.417715
O28	0.296051	0.409202	0.575865	0.541699	0.375042	0.875026	0.193089	0.626086	0.917710
O29	0.106425	0.395166	0.917245	0.374973	0.875160	0.875160	0.084078	0.789814	0.082054
O30	0.090798	0.203949	0.757468	0.624997	0.124998	0.875002	0.249257	0.710185	0.582053
O31	0.711717	0.105736	0.583264	0.458354	0.375139	0.124761	0.026417	0.623911	0.832285
O32	0.892097	0.104844	0.918284	0.377764	0.366603	0.366603	0.306919	0.876087	0.332284
O33	0.893261	0.288978	0.749765	0.708298	0.125052	0.125052	0.415936	0.539834	0.167921
O34	0.788283	0.394264	0.583264	0.708332	0.625048	0.625048	0.584069	0.960006	0.667935
O35	0.607903	0.395156	0.918284	0.875000	0.125003	0.625000	0.473578	0.873914	0.417705
O36	0.606739	0.211022	0.749765	0.875000	0.624999	0.125003	0.526366	0.626141	0.917796
O37	0.211022	0.606739	0.583569	0.958268	0.375053	0.624947	0.417409	0.789825	0.082063
O38	0.393909	0.605817	0.916594	0.958302	0.875050	0.124950	0.582585	0.710141	0.582067
O39	0.394264	0.788283	0.750070	0.791700	0.874947	0.625050	0.359755	0.623911	0.832286
O40	0.288978	0.893261	0.583569	0.791700	0.625050	0.874947	0.640243	0.876076	0.332282
O41	0.106091	0.894183	0.916594	0.791700	0.125053	0.374950	0.749282	0.539883	0.167929
O42	0.105736	0.711717	0.750070	0.958268	0.624947	0.375053	0.917409	0.960184	0.667946
O43	0.711714	0.605530	0.583292	0.875000	0.874997	0.375000	0.806907	0.873913	0.417711
O44	0.894015	0.605933	0.916756	0.875000	0.375001	0.874997	0.859756	0.626084	0.917705
O45	0.894470	0.788286	0.750041	0.708298	0.874948	0.874948	0.750741	0.789828	0.082064
O46	0.788286	0.894470	0.583292	0.958302	0.124950	0.875050	0.915917	0.710183	0.582051
O47	0.605985	0.894067	0.916756	0.791700	0.374950	0.125053	0.693129	0.623958	0.832307
O48	0.605530	0.711714	0.750041	0.708332	0.374952	0.374952	0.973576	0.876084	0.332289

Table S3 The xyz coordinates for transition state structures in Al^{3+}/Li^{+} substituted SiO_2 phases, Al-S-TS1 was the transition state between Al^{3+}/Li^{+} substituted α-quartz and Al^{3+}/Li^{+} substituted β-quartz, Al-S-TS2 was the transition state between Al^{3+}/Li^{+} substituted β-quartz and Al^{3+}/Li^{+} substituted β-cristobalite, Al-S-TS3 was the transition state between Al^{3+}/Li^{+} substituted β-cristobalite and Al^{3+}/Li^{+} substituted α-cristobalite.

Atom	Al-S-TS1			Al-S-TS2			Al-S-TS3		
number	x	y	z	x	y	z	x	y	z
Si1	0.250486	0.000583	-0.000424	0.000514	0.000015	-0.000013	0.095471	0.143963	0.000030
Si2	-0.000058	0.249628	0.332891	0.000510	0.500015	0.499986	0.236291	0.356171	0.498777
Si3	0.249805	0.249918	0.166381	0.167107	0.000012	0.499989	0.070147	0.394071	0.249840
Si4	0.750619	0.000756	-0.000103	0.167107	0.500013	-0.000010	0.262048	0.105103	0.750543
Si5	0.498323	0.247549	0.332551	0.249478	0.249374	0.750627	0.430268	0.143248	0.001258
Si6	0.750307	0.250052	0.166296	0.083853	0.250042	0.250013	0.404957	0.394587	0.249677
Si7	0.249049	0.499157	-0.000449	0.083853	0.749988	0.749959	0.596484	0.106970	0.747488
Si8	0.001394	0.751539	0.332570	0.249478	0.750652	0.249349	0.762335	0.144539	0.000238
Si9	0.249625	0.749877	0.166399	0.332295	0.000020	-0.000023	0.903384	0.356042	0.499884
Si10	0.749645	0.499554	-0.000189	0.499277	0.000306	0.500078	0.735836	0.393768	0.250919
Si11	0.500341	0.751172	0.332358	0.499277	0.499930	-0.000323	0.928841	0.106059	0.749978
Si12	0.750128	0.749995	0.166426	0.583851	0.248353	0.751654	0.095546	0.644082	-0.000045
Si13	0.249685	-0.001482	0.499379	0.415447	0.245624	0.245764	0.237264	0.855963	0.499467
Si14	-0.001296	0.250085	0.834258	0.415451	0.754225	0.754366	0.070367	0.893961	0.250029
Si15	0.750298	0.001122	0.499760	0.583975	0.751882	0.248125	0.262431	0.607007	0.750583
Si16	0.501306	0.249897	0.834209	0.667085	0.000055	-0.000053	0.430118	0.644367	0.000219
Si17	0.749925	0.249070	0.668413	0.667570	0.499953	0.500050	0.571181	0.855910	0.500548
Si18	0.245195	0.501514	0.498150	0.833854	0.000011	0.499989	0.404403	0.893762	0.250314
Si19	0.001097	0.750029	0.833924	0.833854	0.500013	-0.000009	0.596334	0.604343	0.748943
Si20	0.249985	0.750777	0.666443	0.917176	0.250018	0.749983	0.762326	0.643607	0.000332
Si21	0.755626	0.498631	0.498103	0.750520	0.249904	0.249874	0.903722	0.855953	0.500105
Si22	0.498998	0.750290	0.834095	0.750520	0.750127	0.750098	0.737333	0.894106	0.249709
Si23	0.754917	0.756268	0.669255	0.917176	0.750013	0.249988	0.928854	0.605895	0.750020
Al1	0.245418	0.244546	0.669084	0.331652	0.499989	0.500020	0.573279	0.356315	0.498771
Li1	0.500894	0.500456	0.570584	0.491453	0.506405	0.492929	0.421443	0.337902	0.634751
O1	0.211441	0.105270	0.083691	0.041447	0.125184	0.125154	0.082711	0.039894	0.167876
O2	0.395160	0.105268	0.416094	0.041563	0.625160	0.625130	0.251169	0.459600	0.667872
O3	0.394595	0.289247	0.250076	0.207970	0.124206	0.625759	0.140663	0.373842	0.418202

O4	0.288854	0.394859	0.083765	0.207969	0.625790	0.124179	0.193430	0.126136	0.917315
O5	0.104141	0.393802	0.415525	0.290255	0.368572	0.631428	0.084238	0.289798	0.082045
O6	0.105744	0.211669	0.250039	0.291830	0.875624	0.124379	0.249603	0.210518	0.582010
O7	0.710878	0.105063	0.083812	0.124762	0.875133	0.624799	0.026747	0.123954	0.832548
O8	0.893998	0.105714	0.416456	0.124762	0.624828	0.875108	0.306762	0.375908	0.333062
O9	0.894245	0.288434	0.250169	0.124762	0.124894	0.375174	0.415745	0.040079	0.167677
O10	0.788760	0.394728	0.083839	0.290266	0.631460	0.368540	0.583858	0.463952	0.673490
O11	0.603863	0.396026	0.419005	0.207969	0.875822	0.374212	0.469553	0.374483	0.414343
O12	0.606549	0.212539	0.250270	0.207970	0.374243	0.875796	0.525647	0.126233	0.918600
O13	0.212013	0.605713	0.083550	0.041447	0.874847	0.874818	0.417177	0.289851	0.081421
O14	0.396755	0.606203	0.417869	0.291827	0.124408	0.875595	0.582252	0.205349	0.586060
O15	0.393851	0.788269	0.249963	0.124762	0.375202	0.124869	0.359761	0.124512	0.831377
O16	0.288370	0.894544	0.083505	0.041563	0.374872	0.374842	0.642757	0.376830	0.326967
O17	0.105644	0.892543	0.415638	0.375597	0.123448	0.123415	0.749301	0.039618	0.168038
O18	0.105360	0.710841	0.249848	0.378271	0.628027	0.627846	0.917588	0.460268	0.668042
O19	0.711627	0.605515	0.083531	0.541738	0.127046	0.624037	0.807550	0.373858	0.418161
O20	0.895135	0.606997	0.416054	0.541666	0.623993	0.127408	0.860045	0.125974	0.917428
O21	0.893881	0.787892	0.250203	0.624185	0.375853	0.624147	0.751047	0.289365	0.081400
O22	0.788074	0.894406	0.083504	0.625093	0.875487	0.124514	0.916072	0.210076	0.582151
O23	0.606161	0.893997	0.417111	0.459351	0.872768	0.624867	0.693165	0.123705	0.832675
O24	0.605828	0.711249	0.250435	0.459335	0.625103	0.872893	0.973992	0.376122	0.331987
O25	0.207829	0.097089	0.577548	0.459337	0.127127	0.374902	0.082720	0.539790	0.167970
O26	0.394422	0.104986	0.917469	0.624120	0.624135	0.375864	0.250827	0.960499	0.668146
O27	0.406151	0.295781	0.752531	0.541666	0.872600	0.376002	0.140435	0.873904	0.417936
O28	0.298184	0.406716	0.577547	0.541738	0.375959	0.872963	0.193331	0.625937	0.917369
O29	0.105175	0.395067	0.917629	0.375597	0.876585	0.876552	0.084187	0.789784	0.082025
O30	0.095613	0.207793	0.754875	0.625071	0.124603	0.875398	0.249293	0.709929	0.582217
O31	0.711426	0.105677	0.582964	0.459354	0.375137	0.127250	0.026721	0.623948	0.832532
O32	0.892552	0.105611	0.917772	0.378274	0.372159	0.371978	0.306796	0.876113	0.332439
O33	0.893622	0.289442	0.750250	0.708081	0.125232	0.125225	0.415687	0.539583	0.167863
O34	0.788569	0.394023	0.583833	0.708224	0.625363	0.625301	0.583939	0.959708	0.668046
O35	0.607448	0.394608	0.917457	0.874720	0.125233	0.625195	0.473200	0.874017	0.417282
O36	0.606491	0.211146	0.749898	0.874718	0.625225	0.125203	0.525763	0.626393	0.918555
O37	0.210802	0.606620	0.583396	0.957907	0.375311	0.624691	0.417247	0.789835	0.082012
O38	0.394251	0.605725	0.916642	0.958038	0.875264	0.124737	0.582442	0.710678	0.581828

O39	0.394512	0.788046	0.749503	0.791465	0.875123	0.624777	0.359544	0.623481	0.831772
O40	0.289281	0.893163	0.582587	0.791464	0.624804	0.875098	0.640148	0.876077	0.332309
O41	0.105680	0.894004	0.916924	0.791464	0.124904	0.375198	0.749542	0.540373	0.167386
O42	0.105266	0.711281	0.749868	0.957900	0.624714	0.375288	0.917521	0.960178	0.667930
O43	0.709313	0.604752	0.582895	0.874718	0.874798	0.374777	0.807074	0.873890	0.417869
O44	0.894060	0.606241	0.916593	0.874720	0.374806	0.874769	0.860039	0.626120	0.917407
O45	0.895199	0.787717	0.750242	0.708081	0.874777	0.874769	0.750779	0.789967	0.082141
O46	0.787737	0.893784	0.582316	0.958039	0.124766	0.875235	0.916033	0.710218	0.582031
O47	0.606261	0.893885	0.916555	0.791465	0.375225	0.124878	0.693219	0.624228	0.832533
O48	0.604010	0.709228	0.747701	0.708224	0.374700	0.374639	0.973826	0.876128	0.332063

Table S4 The xyz coordinates for transition state structures in $4H^+$ substituted SiO_2 phases, H-S-TS1 was the transition state between $4H^+$ substituted α-quartz and $4H^+$ substituted β-quartz, H-S-TS2 was the transition state between $4H^+$ substituted β-quartz and $4H^+$ substituted β-cristobalite, H-S-TS3 was the transition state between $4H^+$ substituted β-cristobalite and $4H^+$ substituted α-cristobalite.

Atom	H-S-TS1			H-S-TS2			H-S-TS3		
number	x	y	z	x	y	z	x	y	z
Si1	0.250515	0.000512	0.000381	-0.000045	-0.000036	-0.000036	0.095789	0.143981	-0.000041
Si2	0.000474	0.250218	0.333241	-0.000017	0.499923	0.499923	0.237012	0.355676	0.499589
Si3	0.249453	0.249393	0.166467	0.166531	0.000274	0.499656	0.070496	0.394016	0.250029
Si4	0.749342	0.000288	0.000516	0.166531	0.499656	0.000274	0.262584	0.105916	0.750106
Si5	0.501587	0.250394	0.332445	0.249779	0.249538	0.750794	0.429690	0.143387	0.000121
Si6	0.749708	0.249250	0.166411	0.083428	0.250055	0.250055	0.403403	0.394110	0.248622
Si7	0.249810	0.500512	0.000038	0.083358	0.750037	0.750037	0.596155	0.106364	0.749317
Si8	-0.000130	0.749339	0.332333	0.249779	0.750794	0.249538	0.762412	0.144189	0.000010
Si9	0.249621	0.749043	0.166598	0.333143	0.000971	0.000971	0.903696	0.355897	0.499845
Si10	0.749779	0.500415	0.000467	0.499982	0.000494	0.499219	0.736825	0.393637	0.250352
Si11	0.501002	0.750547	0.332867	0.499982	0.499219	0.000494	0.929111	0.106120	0.749977
Si12	0.749372	0.749348	0.166565	0.583392	0.250011	0.750051	0.095741	0.644010	0.000088
Si13	0.249923	-0.002772	0.495866	0.416577	0.250406	0.250406	0.237274	0.856125	0.499847
Si14	-0.002949	0.252139	0.834203	0.417773	0.753307	0.753307	0.070585	0.894107	0.250022
Si15	0.750191	0.000553	0.500204	0.583392	0.750051	0.250011	0.262214	0.606268	0.750011
Si16	0.499070	0.253760	0.828274	0.666611	-0.000050	-0.000050	0.429283	0.644467	0.000833
Si17	0.748893	0.248966	0.666151	0.666641	0.499918	0.499918	0.570855	0.856731	0.499918
Si18	0.246522	0.507992	0.498968	0.833294	-0.000061	0.499938	0.404138	0.894368	0.250203
Si19	0.000216	0.749707	0.833318	0.833294	0.499938	-0.000061	0.596500	0.608838	0.752156
Si20	0.249918	0.750526	0.667711	0.916713	0.250019	0.750019	0.762865	0.643771	0.000998
Si21	0.749795	0.500577	0.500160	0.750052	0.250017	0.250017	0.903936	0.856006	0.500071
Si22	0.500850	0.750021	0.833372	0.750048	0.750020	0.750020	0.737425	0.894390	0.249878
Si23	0.749614	0.749548	0.666641	0.916713	0.750019	0.250019	0.929208	0.605894	0.749842
H1	0.137579	0.164395	0.821789	0.300479	0.491396	0.692641	0.517704	0.437664	0.663173
H2	0.313993	0.360553	0.498980	0.300479	0.692641	0.491396	0.451827	0.427366	0.535006
H3	0.235132	0.068263	0.664017	0.330937	0.653155	0.653155	0.553847	0.294301	0.634156
H4	0.380254	0.316451	0.670441	0.401083	0.456163	0.456163	0.630765	0.438812	0.447259
O1	0.211149	0.105232	0.083143	0.041687	0.124929	0.124929	0.082642	0.039794	0.167946

O2	0.394800	0.105688	0.415732	0.041736	0.624918	0.624918	0.250810	0.460201	0.667979
O3	0.394476	0.288996	0.250549	0.208408	0.124585	0.624996	0.140346	0.373946	0.417803
O4	0.288898	0.395030	0.083534	0.208408	0.624996	0.124585	0.193148	0.126107	0.917654
O5	0.105673	0.394831	0.415575	0.291420	0.381137	0.631271	0.084147	0.289822	0.082059
O6	0.105569	0.211518	0.250071	0.291660	0.875249	0.123959	0.249330	0.210314	0.582082
O7	0.711086	0.105360	0.083713	0.125030	0.874985	0.625062	0.026529	0.123905	0.832375
O8	0.893638	0.105191	0.416546	0.125030	0.625062	0.874985	0.306633	0.376222	0.332316
O9	0.894362	0.288895	0.249664	0.124948	0.125018	0.374974	0.415798	0.039742	0.167919
O10	0.789182	0.395026	0.083591	0.291420	0.631271	0.381137	0.581130	0.459477	0.669570
O11	0.604707	0.394345	0.416868	0.208063	0.875896	0.375293	0.472181	0.376291	0.423951
O12	0.605754	0.211437	0.249814	0.208063	0.375293	0.875896	0.526052	0.126093	0.918607
O13	0.211694	0.605444	0.083457	0.041680	0.875031	0.875031	0.417526	0.290211	0.082417
O14	0.393684	0.606458	0.415709	0.291660	0.123959	0.875249	0.580951	0.212277	0.585924
O15	0.394299	0.789042	0.249704	0.124948	0.374974	0.125018	0.359711	0.124081	0.832328
O16	0.288788	0.894335	0.083682	0.041734	0.375033	0.375033	0.640814	0.379720	0.335526
O17	0.104851	0.892802	0.414818	0.374992	0.124920	0.124920	0.749306	0.039585	0.168027
O18	0.105313	0.711323	0.250112	0.372650	0.628552	0.628552	0.917328	0.460315	0.668084
O19	0.711666	0.605352	0.083356	0.541687	0.124856	0.625070	0.807447	0.374029	0.417926
O20	0.894348	0.605721	0.416655	0.541687	0.625070	0.124856	0.859880	0.126038	0.917663
O21	0.894661	0.788802	0.249904	0.624998	0.374974	0.624950	0.750794	0.289664	0.081791
O22	0.788820	0.894599	0.083548	0.624992	0.874987	0.124970	0.916051	0.210145	0.582145
O23	0.606132	0.894573	0.416853	0.458360	0.874443	0.624774	0.693295	0.123572	0.832855
O24	0.605557	0.711244	0.249940	0.458360	0.624774	0.874443	0.973787	0.376116	0.332224
O25	0.211789	0.094334	0.585320	0.458727	0.123918	0.375029	0.082667	0.539841	0.167894
O26	0.395046	0.107812	0.915008	0.624998	0.624950	0.374974	0.250763	0.960162	0.667937
O27	0.398809	0.289652	0.748253	0.541729	0.874741	0.375183	0.140324	0.873877	0.417755
O28	0.293164	0.397972	0.570254	0.541729	0.375183	0.874741	0.193228	0.626063	0.917625
O29	0.104312	0.394809	0.917792	0.374707	0.874888	0.874888	0.084141	0.789780	0.082029
O30	0.100048	0.206077	0.759817	0.624992	0.124970	0.874987	0.249335	0.710056	0.582173
O31	0.711205	0.105647	0.583372	0.458727	0.375029	0.123918	0.026524	0.623935	0.832382
O32	0.893430	0.106135	0.918196	0.377692	0.378261	0.378261	0.306919	0.876015	0.332299
O33	0.894450	0.290307	0.748594	0.708294	0.125021	0.125021	0.415849	0.539960	0.167492
O34	0.789140	0.394301	0.583606	0.708318	0.625009	0.625009	0.584120	0.959533	0.667842
O35	0.605331	0.392952	0.916789	0.874991	0.124972	0.624976	0.473498	0.873690	0.417627
O36	0.606266	0.210350	0.750537	0.874991	0.624976	0.124972	0.526132	0.626020	0.917631

O37	0.209434	0.608237	0.585973	0.958299	0.375040	0.624938	0.417386	0.789656	0.081893
O38	0.394368	0.606143	0.917078	0.958295	0.875019	0.124929	0.582518	0.709660	0.582180
O39	0.394599	0.788630	0.749863	0.791699	0.874900	0.625032	0.359952	0.623627	0.831932
O40	0.289434	0.893779	0.583429	0.791699	0.625032	0.874900	0.640183	0.875744	0.332397
O41	0.105705	0.895231	0.915708	0.791704	0.125037	0.374930	0.749620	0.540589	0.167143
O42	0.105543	0.711243	0.749828	0.958299	0.624938	0.375040	0.917458	0.960135	0.667901
O43	0.711346	0.605486	0.583358	0.875000	0.875009	0.374983	0.806935	0.873839	0.417710
O44	0.894110	0.605391	0.917221	0.875000	0.374983	0.875009	0.859766	0.626163	0.917498
O45	0.894658	0.788895	0.749701	0.708287	0.874936	0.874936	0.750689	0.789747	0.081839
O46	0.788529	0.894214	0.583203	0.958295	0.124929	0.875019	0.915960	0.710202	0.582086
O47	0.605220	0.893689	0.916389	0.791704	0.374930	0.125037	0.692847	0.623621	0.831480
O48	0.605451	0.711533	0.750008	0.708357	0.374933	0.374933	0.973662	0.876079	0.332244

Table S5 The lattice parameters for transition state structures in Tables S1-S4

Structure	Lattice parameters					
	a **(Å)**	***b*** **(Å)**	***c*** **(Å)**	**α (º)**	**β (º)**	**γ (º)**
TS1	10.169	10.169	11.225	90.000	90.000	119.922
TS2	22.263	7.420	7.420	90.000	90.000	90.000
TS3	15.104	10.070	7.051	90.000	90.000	90.000
Ti-S-TS1	10.231	10.231	11.241	90.000	90.000	120.305
Ti-S-TS2	22.374	7.459	7.459	90.001	90.000	90.000
Ti-S-TS3	15.466	10.309	7.170	90.062	89.935	90.015
Al-S-TS1	10.289	10.210	11.165	89.967	90.065	120.217
Al-S-TS2	22.223	7.442	7.442	90.150	89.999	90.000
Al-S-TS3	15.460	10.288	7.180	90.108	90.132	90.001
H-S-TS1	10.251	10.261	11.204	89.804	90.161	120.609
H-S-TS2	22.366	7.466	7.466	90.067	90.075	90.075
H-S-TS3	15.449	10.283	7.155	90.094	90.009	90.089