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Supporting information for article:

Communication between cation environments in aluminosilicate frameworks: incommensurately modulated crystal structure of an *e*-plagioclase

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Table S1a: EPMA data for the *e*-plagioclase crystal (a) in wt. %.

oxide %							
Line #	Na_2O	K_2O	CaO	FeO	SiO_2	Al_2O_3	Total
348 G	5.903	0.776	8.982	0.232	56.488	27.149	99.530
349 G	5.734	0.974	9.037	0.164	56.068	27.204	99.181
350 G	5.853	0.950	8.986	0.418	56.321	27.084	99.612
351 G	5.828	0.845	9.012	0.210	57.108	27.002	100.005
352 G	5.962	0.841	9.014	0.312	56.338	26.892	99.359
353 G	5.843	0.833	8.895	0.454	56.603	27.042	99.670
354 G	5.909	0.681	8.945	0.537	56.891	27.167	100.130
357 G	5.697	1.054	8.983	0.697	56.069	26.626	99.126
358 G	5.706	1.083	8.995	0.213	56.054	26.877	98.928
359 G	5.554	1.039	8.919	0.203	56.426	26.861	99.002
360 G	5.705	1.143	8.844	0.273	56.929	26.954	99.848
361 G	5.720	1.191	8.991	0.348	56.211	26.728	99.189
362 G	5.748	0.893	9.102	0.229	56.530	26.932	99.434
363 G	5.811	0.823	9.249	0.274	56.559	26.624	99.340
364 G	5.854	0.784	9.004	0.225	56.748	27.171	99.786
365 G	6.038	0.716	8.910	0.260	56.330	27.245	99.499
366 G	6.032	0.821	9.045	0.224	56.773	27.001	99.896
367 G	5.898	0.805	9.128	0.289	56.714	27.356	100.190
368 G	5.889	0.788	9.134	0.251	56.566	27.040	99.668
369 G	5.824	0.741	9.009	0.268	56.613	26.894	99.349
371 G	5.590	0.793	9.113	0.245	56.264	26.865	98.870
372 G	6.112	0.779	9.033	0.263	56.237	27.233	99.657
373 G	5.786	1.100	9.163	0.197	56.740	27.229	100.215
374 G	5.762	0.874	9.170	0.481	56.205	26.977	99.469
375 G	5.851	1.028	9.107	0.257	56.736	26.808	99.787
376 G	5.823	0.825	9.015	0.307	57.158	27.195	100.323
377 G	5.947	0.725	9.026	0.231	56.286	27.121	99.336
378 G	5.970	0.968	8.979	0.463	56.402	26.725	99.507
379 G	5.950	0.818	9.225	0.228	56.413	27.025	99.659
380 G	5.844	0.875	8.769	0.247	56.568	26.731	99.034
381 G	5.929	0.782	9.060	0.297	56.346	27.142	99.556
382 G	5.411	1.242	8.939	0.276	55.960	26.469	98.297
383 G	5.895	0.832	9.184	0.376	56.224	27.260	99.771
384 G	5.945	0.949	9.100	0.255	56.382	26.847	99.478
385 G	5.754	1.056	8.920	0.391	56.021	26.957	99.099
Average	5.831(14)	0.898(14)	9.028(11)	0.303(11)	56.465(30)	26.984(21)	99.509(43)

Table S1b: EPMA data for the *e*-plagioclase calculated based on 8 oxygen atoms per oxigen unit.

Point #	Na	K	Ca	Fe	Si	Al	O
348 G	0.517	0.045	0.435	0.009	2.553	1.446	8
349 G	0.505	0.056	0.440	0.006	2.546	1.456	8
350 G	0.514	0.055	0.436	0.016	2.549	1.445	8
351 G	0.508	0.048	0.434	0.008	2.567	1.430	8
352 G	0.524	0.049	0.438	0.012	2.554	1.437	8
353 G	0.512	0.048	0.430	0.017	2.556	1.439	8
354 G	0.515	0.039	0.431	0.020	2.557	1.439	8
357 G	0.503	0.061	0.439	0.027	2.555	1.430	8
358 G	0.504	0.063	0.439	0.008	2.553	1.443	8
359 G	0.489	0.060	0.434	0.008	2.563	1.438	8
360 G	0.499	0.066	0.427	0.010	2.566	1.432	8
361 G	0.504	0.069	0.438	0.013	2.557	1.433	8
362 G	0.504	0.051	0.441	0.009	2.559	1.437	8
363 G	0.511	0.048	0.449	0.010	2.563	1.422	8
364 G	0.512	0.045	0.435	0.008	2.557	1.443	8
365 G	0.529	0.041	0.432	0.010	2.547	1.452	8
366 G	0.527	0.047	0.437	0.008	2.558	1.434	8
367 G	0.514	0.046	0.439	0.011	2.548	1.449	8
368 G	0.516	0.045	0.442	0.009	2.555	1.439	8
369 G	0.511	0.043	0.437	0.010	2.563	1.435	8
371 G	0.493	0.046	0.444	0.009	2.559	1.440	8
372 G	0.536	0.045	0.438	0.010	2.543	1.451	8
373 G	0.505	0.063	0.442	0.007	2.552	1.443	8
374 G	0.506	0.050	0.445	0.018	2.548	1.441	8
375 G	0.512	0.059	0.441	0.010	2.562	1.427	8
376 G	0.506	0.047	0.433	0.012	2.562	1.437	8
377 G	0.522	0.042	0.438	0.009	2.550	1.448	8
378 G	0.525	0.056	0.436	0.018	2.557	1.428	8
379 G	0.522	0.047	0.447	0.009	2.550	1.440	8
380 G	0.514	0.051	0.427	0.009	2.568	1.430	8
381 G	0.520	0.045	0.439	0.011	2.548	1.447	8
382 G	0.481	0.073	0.439	0.011	2.565	1.430	8
383 G	0.516	0.048	0.445	0.014	2.541	1.452	8
384 G	0.522	0.055	0.442	0.010	2.555	1.434	8
385 G	0.508	0.061	0.435	0.015	2.549	1.446	8
Average	0.512	0.052	0.438	0.011	2.555	1.439	8

Table S2: Atomic coordinates of the average *e*-plagioclase structure in $C\bar{1}$.

Symbol	Element	x	y	z	U_{equiv}	Occupancy
M_a	Ca	0.76945(19)	0.02630(15)	0.1061(3)	0.0268(4)	0.3513
	Na	0.76945(19)	0.02630(15)	0.1061(3)	0.0268(4)	0.1665
M_b	Ca	0.7685(3)	0.9739(2)	0.1715(4)	0.0268(4)	0.1060
	Na	0.7685(3)	0.9739(2)	0.1715(4)	0.0268(4)	0.3762
T_1o	Si	0.99349(10)	0.33473(6)	0.78632(12)	0.0148(3)	0.3766
	Al	0.99349(10)	0.33473(6)	0.78632(12)	0.0148(3)	0.6233
T_2o	Si	0.31341(9)	0.39045(5)	0.68298(11)	0.0125(3)	0.7237
	Al	0.31341(9)	0.39045(5)	0.68298(11)	0.0125(3)	0.2763
T_1m	Si	0.00325(10)	0.31783(6)	0.23194(11)	0.0141(3)	0.6776
	Al	0.00325(10)	0.31783(6)	0.23194(11)	0.0141(3)	0.3224
T_2m	Si	0.68204(9)	0.37977(6)	0.35698(11)	0.0127(3)	0.6793
	Al	0.68204(9)	0.37977(6)	0.35698(11)	0.0127(3)	0.3207
O_A1	O	0.9973(3)	0.37035(16)	0.0223(3)	0.0253(8)	1
O_A2	O	0.4166(2)	0.50644(14)	0.7215(3)	0.0173(7)	1
O_Bo	O	0.1879(2)	0.39322(15)	0.8100(3)	0.0220(8)	1
O_Bm	O	0.8168(3)	0.35311(16)	0.2457(3)	0.0283(9)	1
O_Co	O	0.9856(3)	0.20624(16)	0.7217(3)	0.0240(8)	1
O_cm	O	0.0159(3)	0.18923(17)	0.2181(3)	0.0278(8)	1
O_Do	O	0.8011(2)	0.39166(15)	0.6154(3)	0.0224(7)	1
O_Dm	O	0.1890(3)	0.36747(15)	0.4311(3)	0.0242(8)	1

Table S3: Anisotropic atomic displacement parameters for average *e*-plagioclase structure in $C\bar{1}$.

Symbol	Elemet	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
M_a	Ca	0.0130(4)	0.0372(7)	0.0248(7)	-0.0001(5)	0.0052(4)	-0.0126(5)
	Na	0.0130(4)	0.0372(7)	0.0248(7)	-0.0001(5)	0.0052(4)	-0.0126(5)
M_b	Ca	0.0130(4)	0.0372(7)	0.0248(7)	-0.0001(5)	0.0052(4)	-0.0126(5)
	Na	0.0130(4)	0.0372(7)	0.0248(7)	-0.0001(5)	0.0052(4)	-0.0126(5)
T_1o	Si	0.0137(4)	0.0204(4)	0.0100(4)	-0.0048(3)	0.0048(3)	0.0020(3)
	Al	0.0137(4)	0.0204(4)	0.0100(4)	-0.0048(3)	0.0048(3)	0.0020(3)
T_2o	Si	0.0119(4)	0.0126(4)	0.0118(4)	0.0007(3)	0.0043(3)	-0.0005(3)
	Al	0.0119(4)	0.0126(4)	0.0118(4)	0.0007(3)	0.0043(3)	-0.0005(3)
T_1m	Si	0.0132(4)	0.0197(4)	0.0087(4)	0.0052(3)	0.0043(3)	0.0002(3)
	Al	0.0132(4)	0.0197(4)	0.0087(4)	0.0052(3)	0.0043(3)	0.0002(3)
T_2m	Si	0.0122(4)	0.0145(4)	0.0110(4)	-0.0011(3)	0.0046(3)	0.0019(3)
	Al	0.0122(4)	0.0145(4)	0.0110(4)	-0.0011(3)	0.0046(3)	0.0019(3)
O_A1	O	0.0292(11)	0.0363(12)	0.0136(10)	0.0009(9)	0.0119(9)	0.0051(9)
O_A2	O	0.0172(9)	0.0178(9)	0.0153(9)	-0.0018(7)	0.0056(8)	0.0025(8)
O_Bo	O	0.0220(10)	0.0225(10)	0.0238(11)	-0.0029(8)	0.0123(9)	0.0002(9)
O_Bm	O	0.0227(11)	0.0279(11)	0.0380(13)	0.0025(9)	0.0175(10)	-0.0021(10)
O_Co	O	0.0214(10)	0.0284(11)	0.0207(11)	-0.0070(8)	0.0077(9)	0.0033(9)
O_cm	O	0.0235(10)	0.0309(12)	0.0194(11)	0.0117(9)	0.0019(9)	-0.0066(9)
O_Do	O	0.0214(10)	0.0275(11)	0.0135(10)	-0.0021(8)	0.0032(8)	0.0015(8)
O_Dm	O	0.0209(10)	0.0268(11)	0.0162(10)	0.0016(8)	0.0008(8)	-0.0028(8)

Table S4: Atomic coordinates of the average *e*-plagioclase structure in *C*1.

Symbol	element	x	y	z	Uequi	occ.
M_{1a}ooo	Ca	0.5870(5)	1.0203(3)	0.0813(6)	0.0174(10)	0.375(5)
M_{1b}ooo	Na	0.5797(4)	0.9754(4)	0.1442(6)	0.0174(10)	0.626(5)
M_{2a}ooc	Ca	0.0474(5)	0.9672(3)	0.8704(6)	0.0323(8)	0.28(3)
	Na	0.0474(5)	0.9672(3)	0.8704(6)	0.0323(8)	0.38(5)
M_{2b}ooc	Ca	0.0399(6)	1.0289(4)	0.7995(8)	0.0323(8)	0.26(3)
	Na	0.0399(6)	1.0289(4)	0.7995(8)	0.0323(8)	0.08(7)
T_1oooo	Si	0.3240(3)	0.15845(16)	0.1937(3)	0.0150(8)	0.3026
	Al	0.3240(3)	0.15845(16)	0.1937(3)	0.0150(8)	0.6974
T_1oooc	Si	0.8109(3)	0.32791(17)	0.7662(3)	0.0151(8)	0.4441
	Al	0.8109(3)	0.32791(17)	0.7662(3)	0.0151(8)	0.5559
T_1mooo	Si	0.3213(3)	0.81053(16)	0.2123(3)	0.0135(7)	0.602
	Al	0.3213(3)	0.81053(16)	0.2123(3)	0.0135(7)	0.398
T_1mooc	Si	0.3148(3)	0.17484(16)	0.7483(3)	0.0154(8)	0.7664
	Al	0.3148(3)	0.17484(16)	0.7483(3)	0.0154(8)	0.2335
T_2oooo	Si	0.0046(3)	0.10228(16)	0.2977(3)	0.0132(7)	0.7122
	Al	0.0046(3)	0.10228(16)	0.2977(3)	0.0132(7)	0.2878
T_2oooc	Si	0.1313(3)	0.38322(15)	0.6636(3)	0.0123(7)	0.7237
	Al	0.1313(3)	0.38322(15)	0.6636(3)	0.0123(7)	0.2763
T_2mooo	Si	0.9995(3)	0.87268(15)	0.3379(3)	0.0129(7)	0.6546
	Al	0.9995(3)	0.87268(15)	0.3379(3)	0.0129(7)	0.3454
T_2mooc	Si	0.6354(3)	0.11321(16)	0.6240(3)	0.0133(7)	0.7056
	Al	0.6354(3)	0.11321(16)	0.6240(3)	0.0133(7)	0.2944
O_A1ooo	O	0.3174(9)	0.1226(5)	0.9587(10)	0.026(2)	1
O_A1ooc	O	0.3115(9)	0.8633(5)	0.0037(11)	0.025(2)	1
O_A2ooo	O	0.9014(8)	0.9865(4)	0.2583(10)	0.019(2)	1
O_A2ooc	O	0.2348(7)	0.4994(4)	0.7019(9)	0.0157(18)	1
$O_B$oooo	O	0.1257(8)	0.0971(4)	0.1649(11)	0.023(2)	1
$O_B$oooc	O	0.0014(8)	0.3837(4)	0.7857(9)	0.0202(19)	1
$O_B$mooo	O	0.1358(9)	0.8486(5)	0.2302(11)	0.026(2)	1
$O_B$mooc	O	0.5021(9)	0.1427(5)	0.7393(11)	0.029(2)	1
$O_C$oooo	O	0.3304(8)	0.2851(4)	0.2542(10)	0.021(2)	1
$O_C$oooc	O	0.8012(9)	0.1973(4)	0.6975(11)	0.027(2)	1
$O_c$mooo	O	0.8322(9)	0.1793(5)	0.2003(11)	0.028(2)	1
$O_C$mooc	O	0.3004(9)	0.3013(5)	0.7638(11)	0.028(2)	1
$O_D$oooo	O	0.5175(9)	0.1006(5)	0.3630(9)	0.025(2)	1

$O_D$oooc	O	0.1199(8)	0.8836(4)	0.5947(9)	0.021(2)	1
$O_D$mooo	O	0.0050(8)	0.3585(5)	0.4076(10)	0.025(2)	1
$O_C$mooc	O	0.3004(9)	0.3013(5)	0.7638(11)	0.028(2)	1

Table S5: Anisotropic atomic displacement parameters for average *e*-plagioclase structure in *C*1.

Symbol	elemet	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
M_{1a}ooo	Na	0.0077(11)	0.0310(17)	0.0134(15)	-0.0013(11)	0.0050(10)	-0.0035(11)
M_{1b}ooo	Ca	0.0077(11)	0.0310(17)	0.0134(15)	-0.0013(11)	0.0050(10)	-0.0035(11)
M_{2a}ooc	Ca, Na	0.0163(10)	0.0337(11)	0.0336(13)	0.0094(8)	0.0015(8)	-0.0176(10)
M_{2b}ooc	Ca, Na	0.0163(10)	0.0337(11)	0.0336(13)	0.0094(8)	0.0015(8)	-0.0176(10)
T_1oooo	Si, Al	0.0160(12)	0.0184(9)	0.0095(10)	-0.0034(8)	0.0044(8)	0.0024(8)
T_1oooc	Si, Al	0.0115(11)	0.0234(10)	0.0107(10)	-0.0061(8)	0.0051(8)	0.0020(8)
T_1mooo	Si, Al	0.0101(10)	0.0217(10)	0.0087(10)	0.0049(8)	0.0042(9)	0.0012(8)
T_1mooc	Si, Al	0.0168(11)	0.0181(9)	0.0096(10)	0.0058(8)	0.0045(9)	-0.0006(8)
T_2oooo	Si, Al	0.0121(9)	0.0144(9)	0.0118(10)	0.0007(7)	0.0042(8)	0.0003(7)
T_2oooc	Si, Al	0.0126(9)	0.0116(9)	0.0119(10)	0.0008(6)	0.0049(8)	-0.0009(7)
T_2oooo	Si, Al	0.0121(9)	0.0144(9)	0.0118(10)	0.0007(7)	0.0042(8)	0.0003(7)
T_2mooo	Si, Al	0.0138(10)	0.0128(8)	0.0121(10)	-0.0018(7)	0.0053(8)	0.0031(8)
T_2mooc	Si, Al	0.0111(9)	0.0173(9)	0.0105(10)	0.0002(7)	0.0040(8)	0.0010(8)
O_A1ooo	O	0.026(3)	0.041(3)	0.010(3)	0.002(3)	0.008(2)	0.005(2)
O_A1ooc	O	0.032(3)	0.034(3)	0.017(3)	-0.001(2)	0.017(2)	0.004(2)
O_A2ooo	O	0.024(3)	0.015(2)	0.021(3)	-0.002(2)	0.013(2)	0.002(2)
O_A2ooc	O	0.012(2)	0.020(2)	0.010(3)	-0.0030(19)	0.0001(19)	0.002(2)
$O_B$oooo	O	0.022(3)	0.020(2)	0.030(3)	-0.0060(19)	0.013(2)	-0.003(2)
$O_B$oooc	O	0.021(3)	0.024(2)	0.018(3)	-0.0019(19)	0.011(2)	0.000(2)
$O_B$mooo	O	0.025(3)	0.026(3)	0.036(4)	0.001(2)	0.022(3)	-0.005(2)
$O_B$mooc	O	0.021(3)	0.026(3)	0.039(4)	0.002(2)	0.013(3)	-0.002(3)
$O_C$oooo	O	0.020(3)	0.024(3)	0.019(3)	-0.011(2)	0.009(2)	-0.002(2)
$O_C$oooc	O	0.024(3)	0.035(3)	0.022(3)	-0.004(3)	0.007(3)	0.009(3)
$O_c$mooo	O	0.023(3)	0.035(3)	0.018(3)	0.011(2)	0.003(2)	-0.003(2)
$O_C$mooc	O	0.025(3)	0.028(3)	0.022(3)	0.012(2)	0.002(2)	-0.011(2)
$O_D$oooo	O	0.019(3)	0.036(3)	0.016(3)	0.001(2)	0.003(2)	0.009(2)
$O_D$oooc	O	0.022(3)	0.022(3)	0.013(3)	-0.005(2)	0.003(2)	-0.005(2)
$O_D$mooo	O	0.017(3)	0.032(3)	0.014(3)	0.000(2)	-0.002(2)	-0.007(2)
$O_D$mooc	O	0.023(3)	0.023(3)	0.020(3)	0.003(2)	0.003(2)	-0.001(2)

Table S6: Atomic coordinates of the modulated *e*-plagioclase structure in $X\bar{1}$.

Symbol	Element	x	y	z	U_{equi}	Occupancy
M	Ca	0.5196(3)	0.02526(16)	0.05231(16)	0.0200(6)	0.4327
	Na	0.5177(4)	0.9812(2)	0.0833(2)	0.0200(6)	0.5673
T_1o	Si	0.24353(11)	0.83471(7)	0.89314(7)	0.0112(3)	0.4062
	Al	0.24353(11)	0.83471(7)	0.89314(7)	0.0112(3)	0.5938
T_1m	Si	0.25320(11)	0.81789(6)	0.11597(6)	0.0110(3)	0.7286
	Al	0.25320(11)	0.81789(6)	0.11597(6)	0.0110(3)	0.2714
T_2o	Si	0.56340(11)	0.89036(6)	0.34148(7)	0.0107(3)	0.778
	Al	0.56340(11)	0.89036(6)	0.34148(7)	0.0107(3)	0.222
T_2m	Si	0.93210(11)	0.87972(6)	0.17847(6)	0.0106(3)	0.7155
	Al	0.93210(11)	0.87972(6)	0.17847(6)	0.0106(3)	0.2845
O_A1	O	0.2472(3)	0.87066(17)	0.01120(16)	0.0200(9)	1
O_A2	O	0.6664(3)	0.00642(15)	0.36062(16)	0.0145(8)	1
O_Bo	O	0.4377(3)	0.89321(17)	0.40501(17)	0.0191(9)	1
O_Bm	O	0.0669(3)	0.85319(18)	0.12290(19)	0.0249(10)	1
O_Co	O	0.2356(3)	0.70602(17)	0.86072(17)	0.0188(8)	1
O_cm	O	0.2665(3)	0.68959(17)	0.10897(17)	0.0195(8)	1
O_Do	O	0.0512(3)	0.89142(16)	0.30762(16)	0.0190(8)	1
O_Dm	O	0.4394(3)	0.86730(17)	0.21580(17)	0.0208(8)	1

Table S7: Anisotropic atomic displacement parameters for modulated *e*-plagioclase structure in $X\bar{1}$.

Symbol	Elemet	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
M	Ca, Na	0.0118(5)	0.0242(9)	0.0200(9)	0.0008(6)	0.0045(6)	-0.0073(6)
T_1o	Si, Al	0.0121(4)	0.0132(4)	0.0090(4)	-0.0021(3)	0.0051(3)	0.0011(3)
T_2o	Si, Al	0.0110(4)	0.0093(4)	0.0107(4)	0.0003(3)	0.0039(3)	0.0004(3)
T_1m	Si, Al	0.0117(4)	0.0131(4)	0.0082(4)	0.0034(3)	0.0045(3)	0.0007(3)
T_2m	Si, Al	0.0111(4)	0.0100(4)	0.0105(4)	0.0005(3)	0.0044(3)	0.0016(3)
O_A1	O	0.0271(12)	0.0238(12)	0.0120(11)	0.0018(10)	0.0111(10)	0.0024(10)
O_A2	O	0.0154(11)	0.0117(10)	0.0149(11)	-0.0003(8)	0.0050(9)	0.0027(9)
O_Bo	O	0.0202(11)	0.0190(11)	0.0210(12)	-0.0025(9)	0.0119(10)	-0.0005(10)
O_Bm	O	0.0202(12)	0.0259(13)	0.0331(14)	0.0034(10)	0.0164(11)	-0.0019(11)
O_Co	O	0.0177(11)	0.0197(11)	0.0184(12)	-0.0032(9)	0.0074(10)	0.0014(10)
O_cm	O	0.0191(11)	0.0180(11)	0.0165(12)	0.0057(9)	0.0040(10)	-0.0024(9)
O_Do	O	0.0186(11)	0.0203(12)	0.0133(11)	0.0016(9)	0.0026(9)	0.0022(9)
O_Dm	O	0.0188(11)	0.0211(12)	0.0141(11)	0.0011(9)	0.0001(9)	-0.0019(9)

Table S8: Selected interatomic distances for the $X\bar{1}$ model.

Atoms		$d_{av.}$	Atoms		$d_{av.}$
M (Ca)	M (Na)	0.741(7)		O_Do	1.696(4)
	O_A2	2.350(5)	T_1m	O_A1	1.652(4)
	O_A1	2.392(5)		O_Bm	1.629(5)
	O_Do	2.488(6)		O_cm	1.654(4)
	O_Bo	2.462(5)		O_Dm	1.649(4)
	O_cm	2.753(5)	T_2o	O_A2	1.665(3)
M (Na)	O_A2	2.350(7)		O_Bo	1.639(5)
	O_A1	2.411(6)		O_cm	1.641(4)
	O_Do	2.422(7)		O_Dm	1.624(4)
	O_Bo	2.517(6)	T_2m	O_A2	1.669(3)
T_1o	O_A1	1.699(4)		O_Bm	1.638(5)
	O_Bo	1.693(4)		O_Co	1.634(4)
	O_Co	1.685(4)		O_Do	1.650(4)

Table S9: Anisotropic atomic displacement parameters for the modulated *e*-plagioclase structure in *X*1.

Symbol	Element	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
M_1ooo	Ca, Na	0.0095(11)	0.1024(19)	0.0571(15)	-0.0032(11)	0.0060(10)	-0.0613(14)
M_2ooc	Ca, Na	0.0109(12)	0.0039(9)	0.0164(11)	-0.0013(7)	0.0071(8)	0.0013(8)
T_1oooo	Si, Al	0.0160(11)	0.0126(8)	0.0092(8)	-0.0021(7)	0.0061(8)	-0.0003(7)
T_1oooc	Si, Al	0.0089(10)	0.0153(8)	0.0109(9)	-0.0018(7)	0.0044(8)	0.0016(7)
T_1mooo	Si, Al	0.0090(10)	0.0135(8)	0.0071(8)	0.0051(6)	0.0028(8)	0.0017(7)
T_1mooc	Si, Al	0.0150(11)	0.0155(8)	0.0116(9)	0.0018(7)	0.0068(8)	-0.0014(7)
T_2oooo	Si, Al	0.0117(9)	0.0101(7)	0.0125(9)	0.0015(6)	0.0053(7)	0.0009(7)
T_2oooc	Si, Al	0.0117(10)	0.0102(7)	0.0092(8)	-0.0005(6)	0.0037(7)	0.0001(7)
T_2mooo	Si, Al	0.0140(10)	0.0122(8)	0.0090(9)	-0.0016(7)	0.0060(8)	0.0006(7)
T_2mooc	Si, Al	0.0099(9)	0.0115(7)	0.0122(9)	0.0016(6)	0.0038(8)	0.0022(7)
O_A1ooo	O	0.019(3)	0.028(3)	0.009(2)	-0.001(2)	0.005(2)	0.002(2)
O_A1ooc	O	0.037(3)	0.018(2)	0.021(3)	0.003(2)	0.019(3)	0.002(2)
O_A2ooo	O	0.024(3)	0.016(2)	0.010(2)	0.0043(18)	0.011(2)	0.0070(18)
O_A2ooc	O	0.010(2)	0.0094(18)	0.020(3)	-0.0071(17)	0.002(2)	-0.0007(19)
$O_B$oooo	O	0.024(3)	0.019(2)	0.015(2)	-0.0058(19)	0.012(2)	-0.0045(19)
$O_B$oooc	O	0.015(3)	0.022(2)	0.029(3)	-0.0015(19)	0.012(2)	0.001(2)
$O_B$mooo	O	0.019(3)	0.028(2)	0.036(4)	0.003(2)	0.021(3)	-0.001(2)
$O_B$mooc	O	0.021(3)	0.027(2)	0.029(3)	0.002(2)	0.012(3)	-0.003(2)
$O_C$oooo	O	0.018(3)	0.013(2)	0.019(2)	-0.0097(18)	0.008(2)	-0.005(2)
$O_c$oooc	O	0.018(3)	0.028(3)	0.019(3)	0.002(2)	0.006(2)	0.006(2)
$O_C$mooo	O	0.015(3)	0.024(2)	0.012(2)	0.0033(19)	0.002(2)	-0.003(2)
$O_c$mooc	O	0.023(3)	0.015(2)	0.025(3)	0.010(2)	0.007(3)	0.001(2)
$O_D$oooo	O	0.019(3)	0.015(2)	0.013(2)	0.0043(19)	0.004(2)	0.001(2)
$O_D$oooc	O	0.018(3)	0.027(2)	0.015(3)	-0.003(2)	0.001(2)	0.002(2)
$O_D$mooo	O	0.015(3)	0.031(3)	0.016(2)	-0.008(2)	0.000(2)	-0.007(2)
$O_D$oooo	O	0.019(3)	0.015(2)	0.013(2)	0.0043(19)	0.004(2)	0.001(2)

Figure S1 Electron density contour viewed in *x*2-*x*3 plane for the M sites from the low temperature data at 100K.

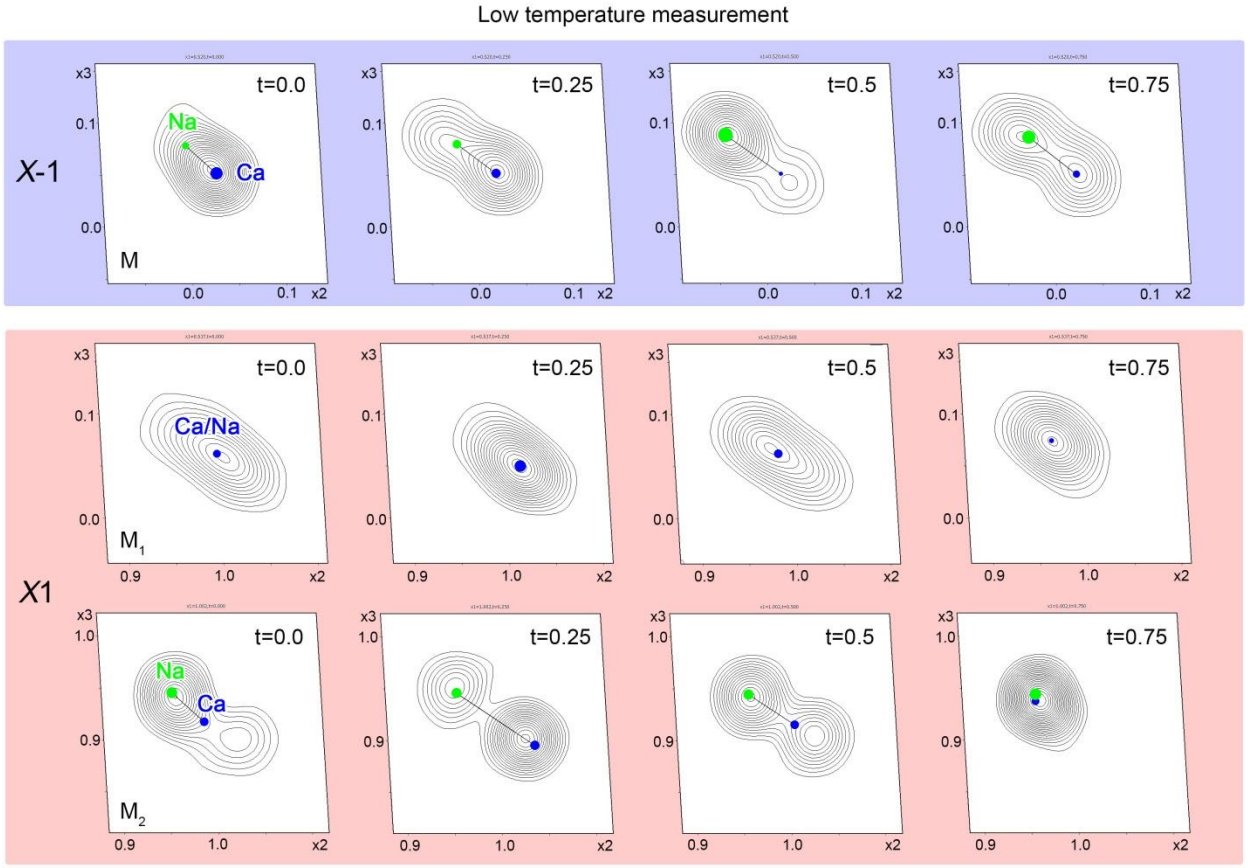


Figure S2 Atomic modeling of the modulated Ca/Na domains for the low temperature measurement at 100K viewed with *x*1-*x*4, *x*2-*x*4, *x*3-*x*4 cross sections.

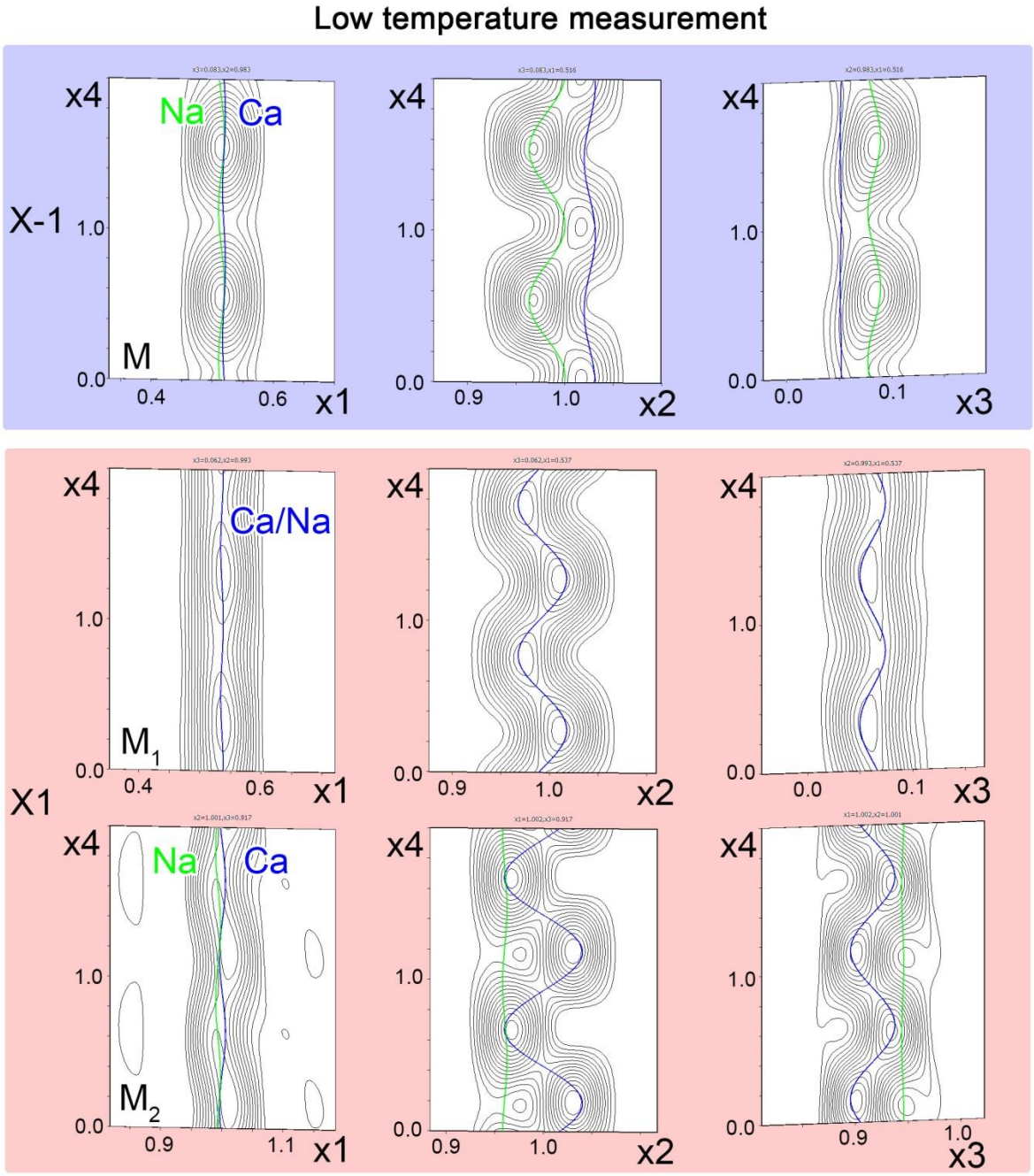


Figure S3 Occupation modulation waves for the a) M site in the $X\bar{1}$ structure, b) M_1 and c) M_2 sites in the $X1$ structure for the low temperature data at 100K.

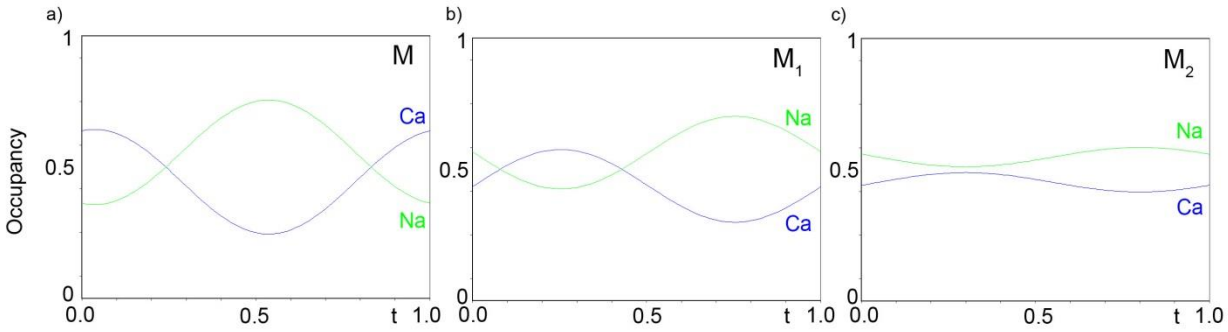


Figure S4 Alternative atomic modeling of the Ca/Na domains for the M_2 site in the $X1$ structure. Crenel functions are employed to model the occupancy modulation of the Ca21, Ca22 positions.

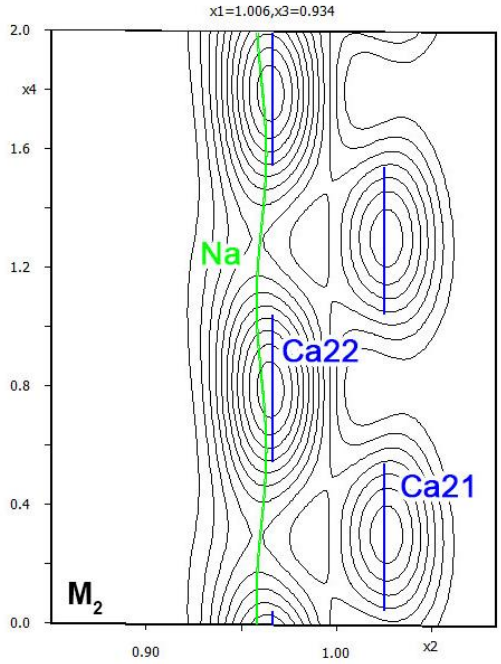
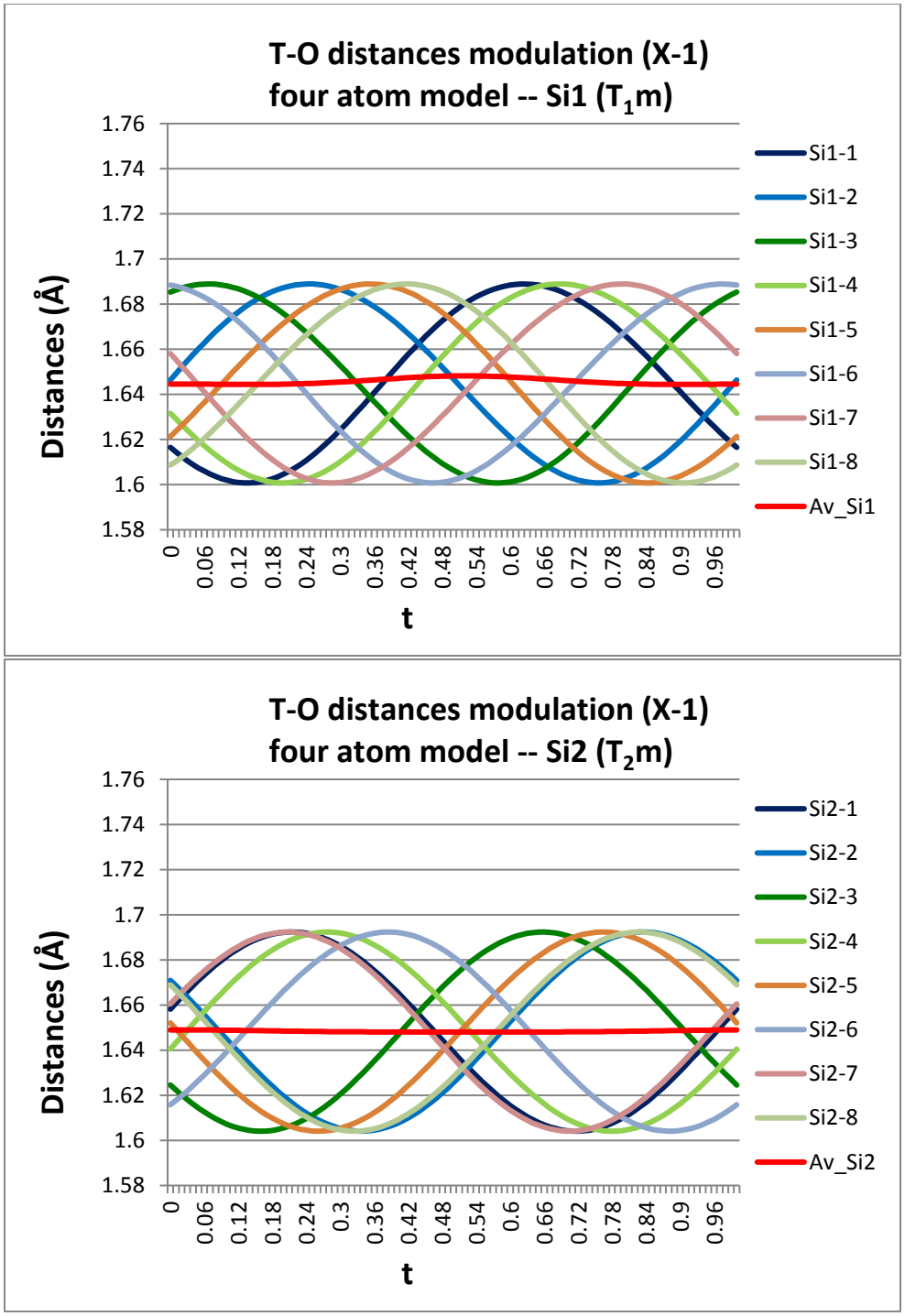
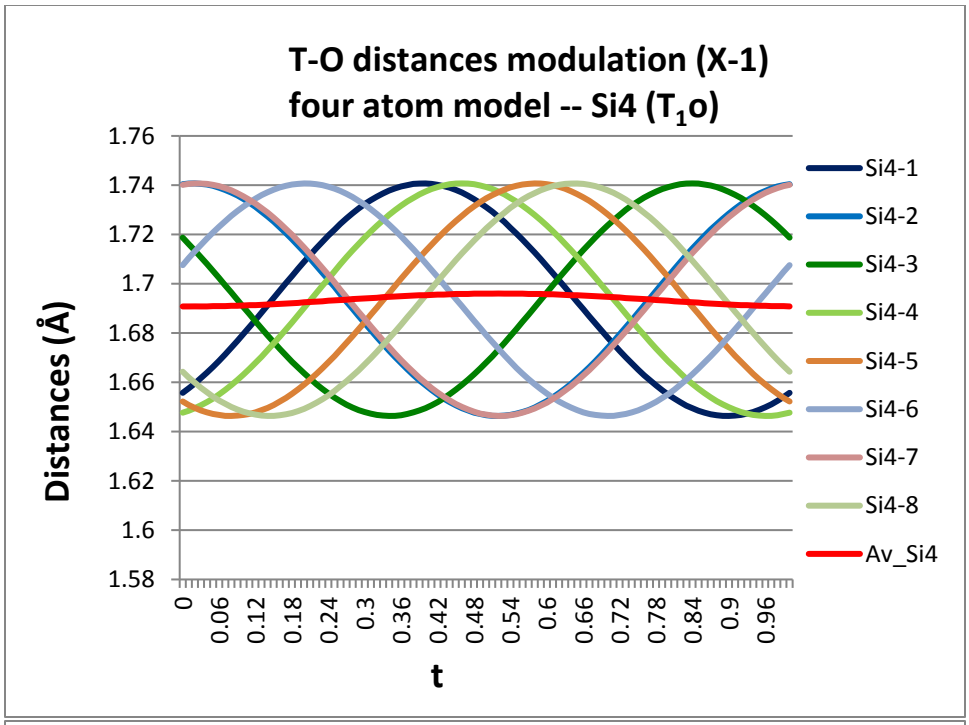


Figure S5 T-O distance modulations in the *X*-1 structure. The modulation curve and average distance at various t-points are shown for each T site.




T-O distances modulation (X-1)
four atom model -- Si4 (T_1o)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si4-1
Si4-2
Si4-3
Si4-4
Si4-5
Si4-6
Si4-7
Si4-8
Av_Si4

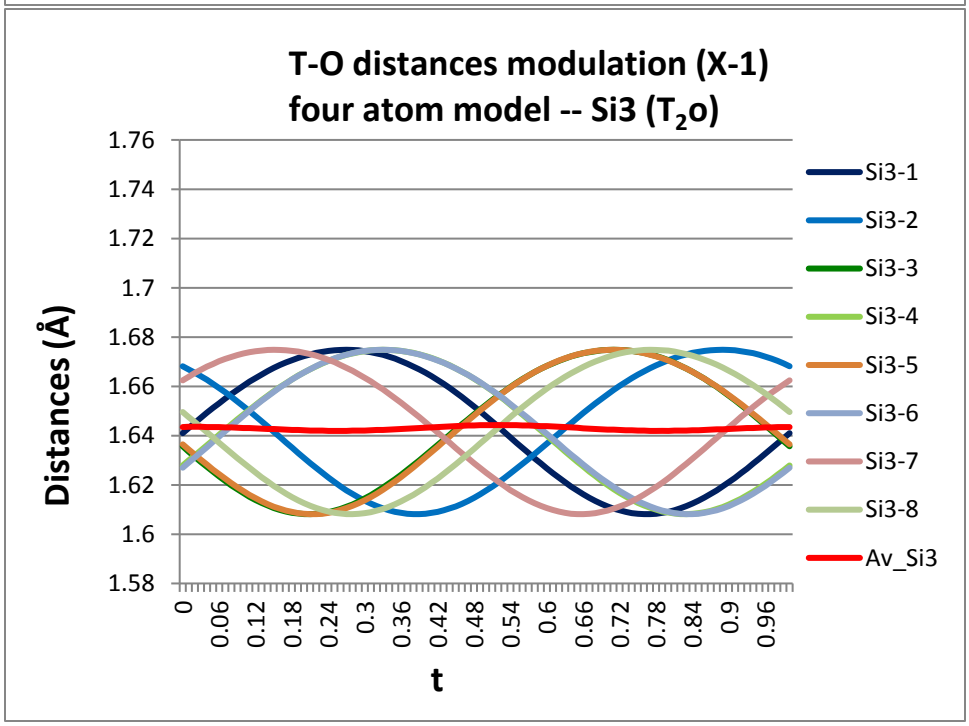
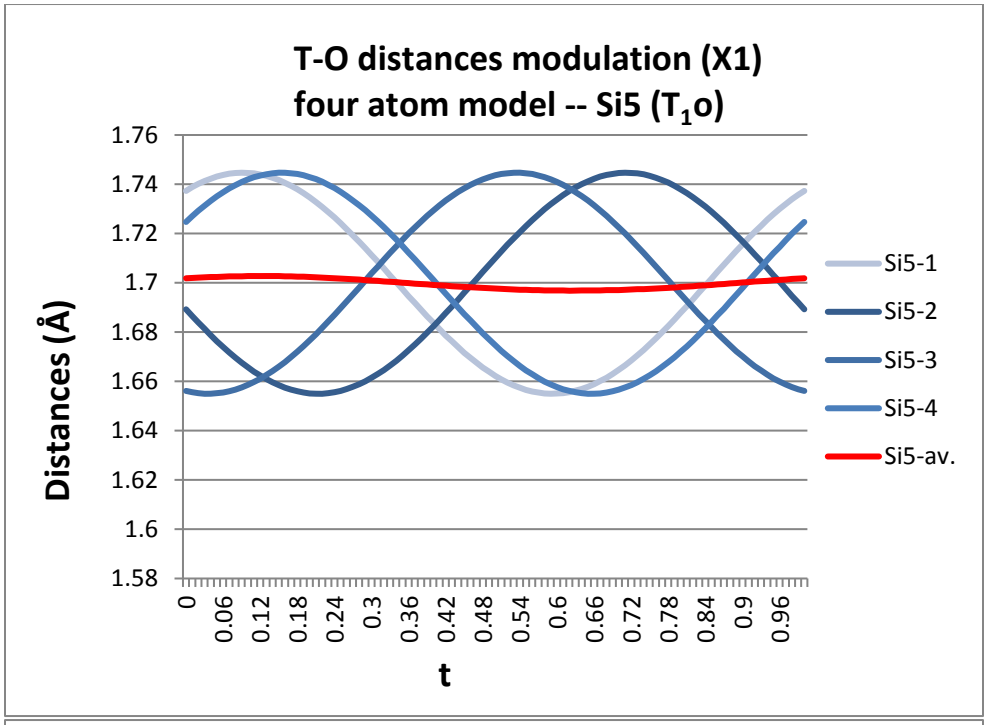
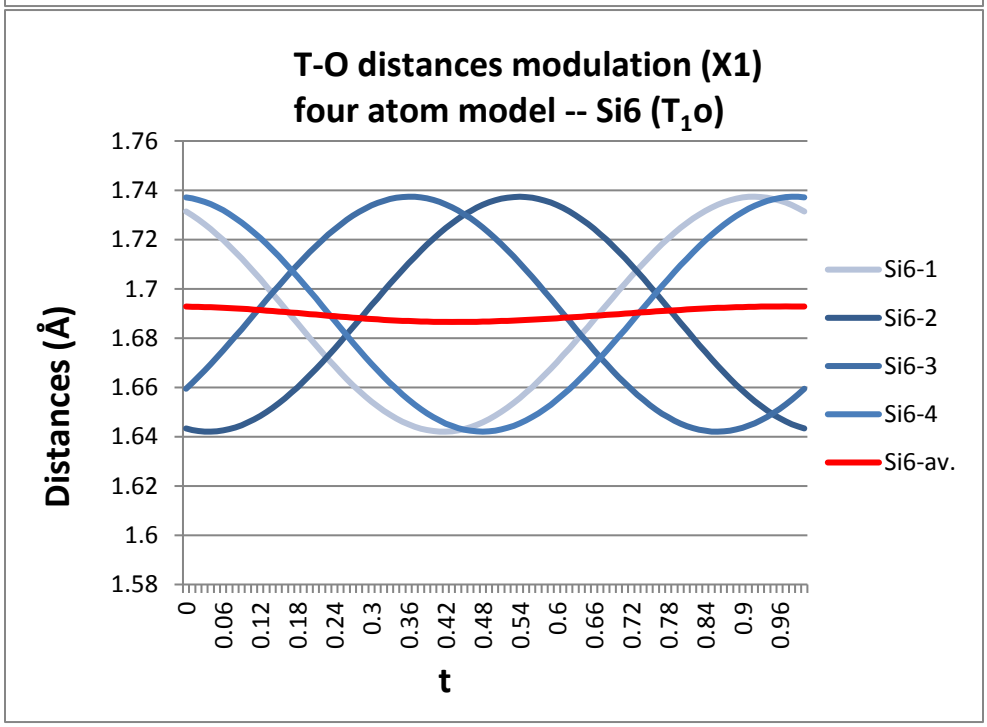
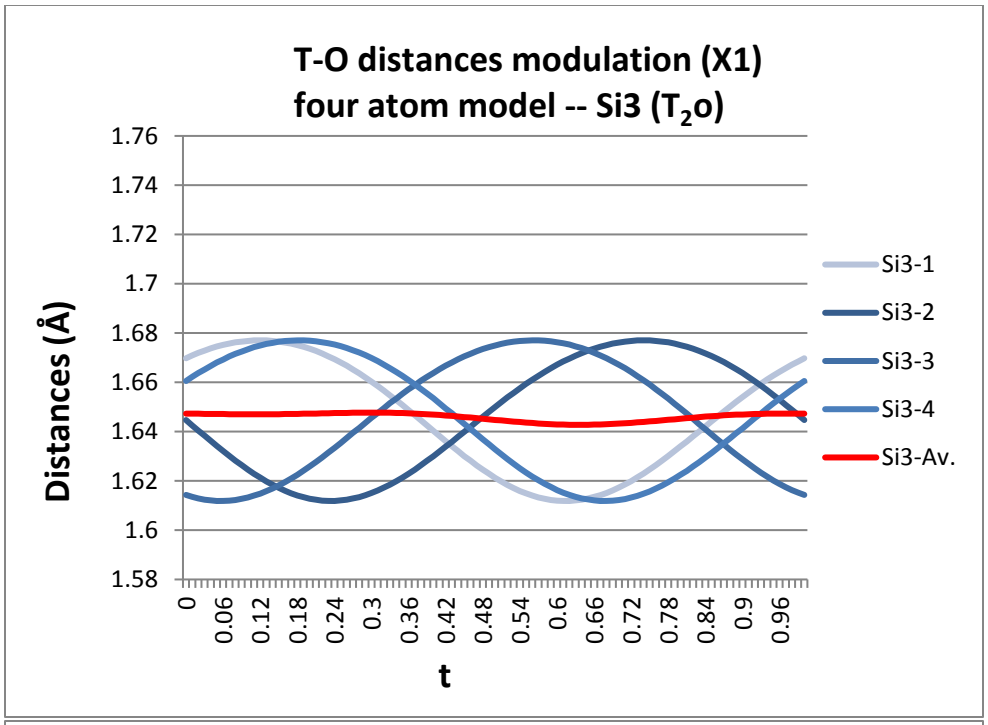
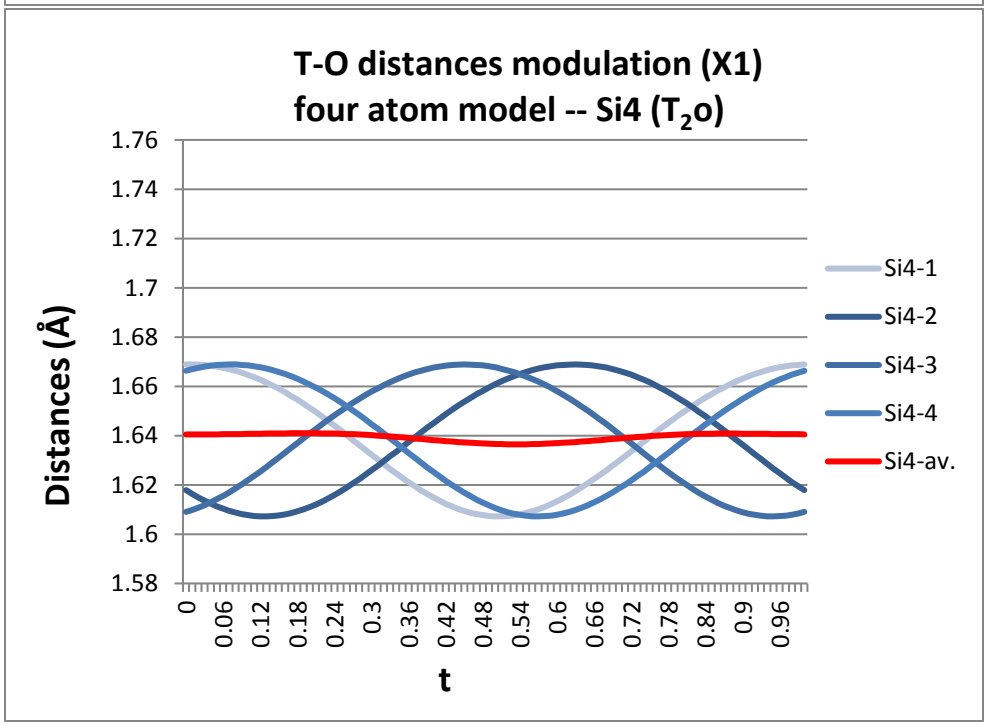

T-O distances modulation (X-1)
four atom model -- Si3 (T_2o)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si3-1
Si3-2
Si3-3
Si3-4
Si3-5
Si3-6
Si3-7
Si3-8
Av_Si3

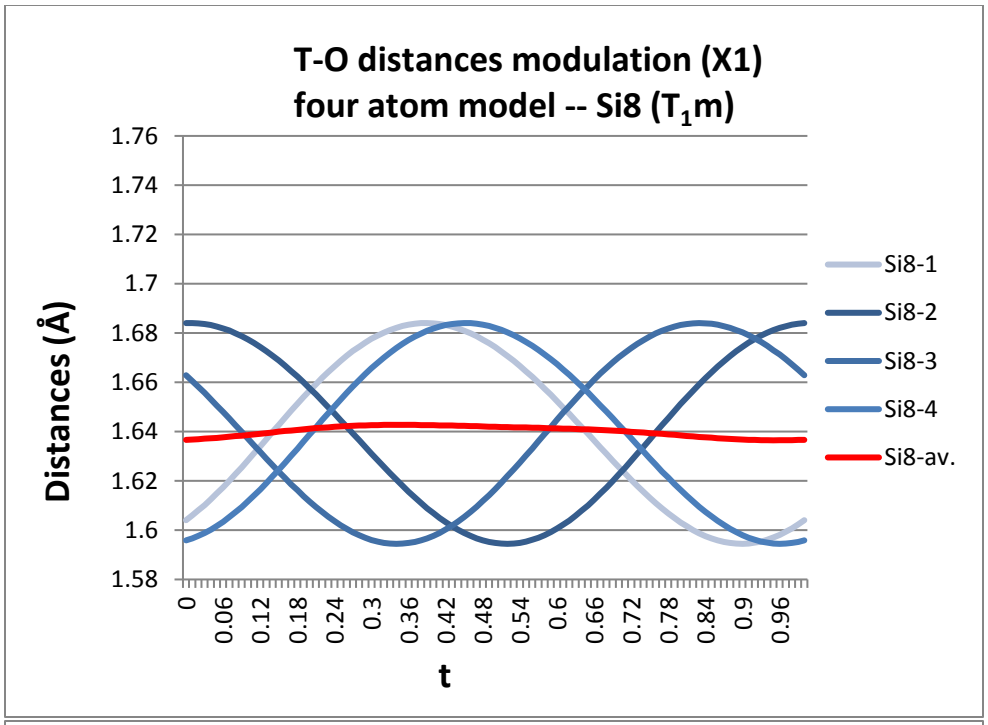
Figure S6 T-O distance modulations in the *X*1 structure. The modulation curve and average distance at various t-points are shown for each T site.

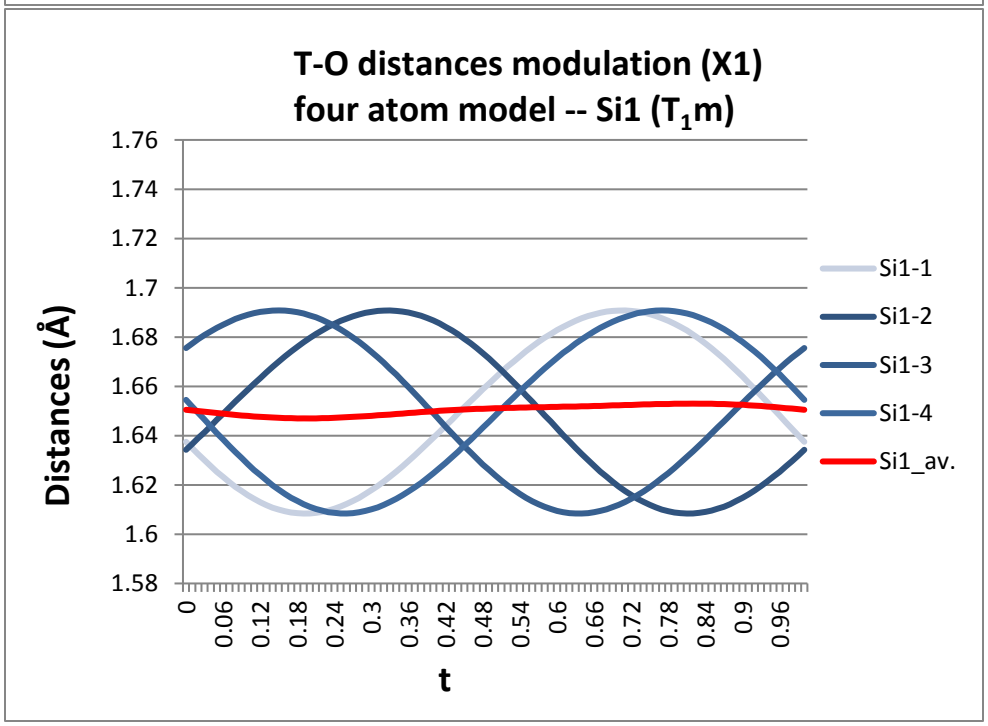


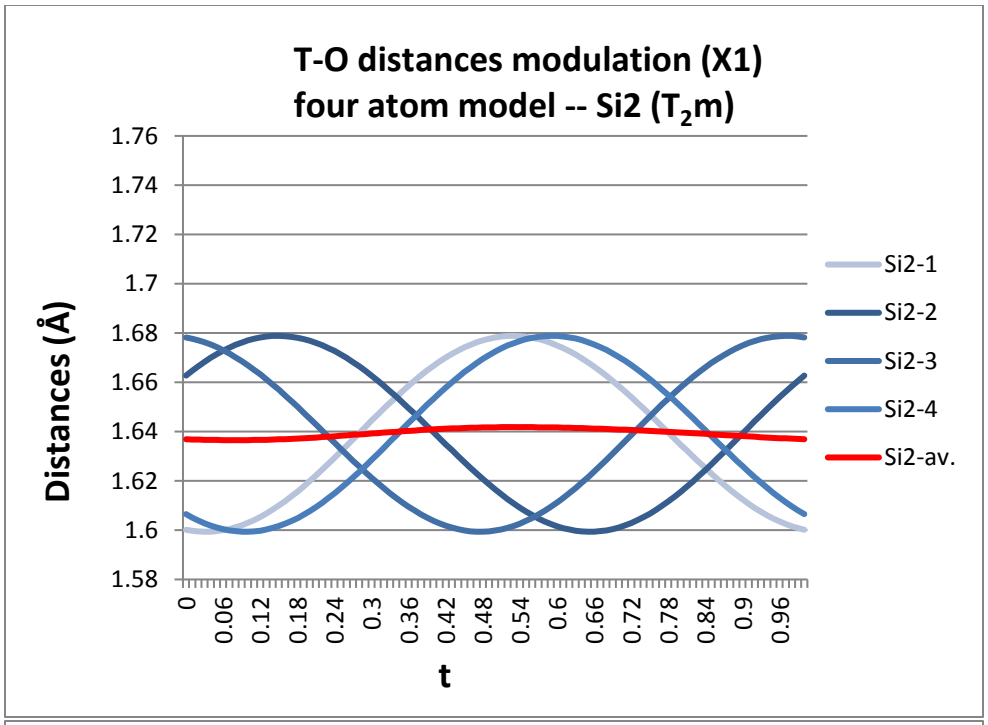


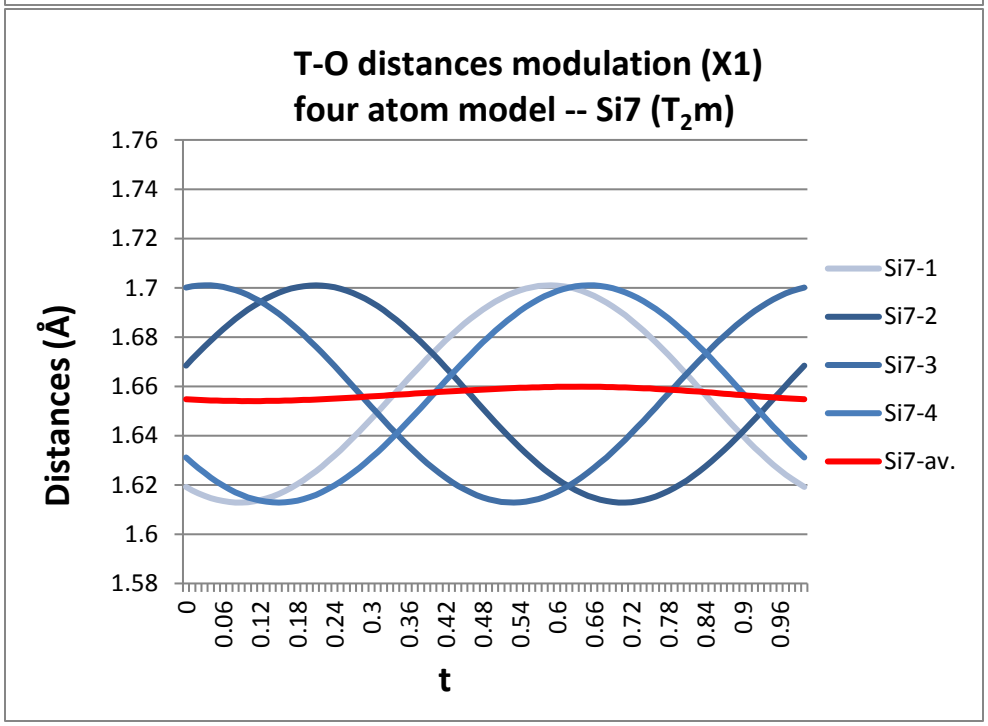

T-O distances modulation (X1)
four atom model -- Si3 (T_2o)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si3-1
Si3-2
Si3-3
Si3-4
Si3-Av.


T-O distances modulation (X1)
four atom model -- Si4 (T_2o)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si4-1
Si4-2
Si4-3
Si4-4
Si4-av.


T-O distances modulation (X1)
four atom model -- Si8 (T_1m)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si8-1
Si8-2
Si8-3
Si8-4
Si8-av.


T-O distances modulation (X1)
four atom model -- Si1 (T_1m)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si1-1
Si1-2
Si1-3
Si1-4
Si1_av.


T-O distances modulation (X1)
four atom model -- Si2 (T_2m)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si2-1
Si2-2
Si2-3
Si2-4
Si2-av.


T-O distances modulation (X1)
four atom model -- Si7 (T_2m)
Distances (Å)
1.76
1.74
1.72
1.7
1.68
1.66
1.64
1.62
1.6
1.58
0
0.06
0.12
0.18
0.24
0.3
0.36
0.42
0.48
0.54
0.6
0.66
0.72
0.78
0.84
0.9
0.96
t
Si7-1
Si7-2
Si7-3
Si7-4
Si7-av.