

Supplementary Material

**Multi-Scale Computational Simulation of Amorphous Silicates.  
Structural, Dielectric and Vibrational Spectroscopic Properties**

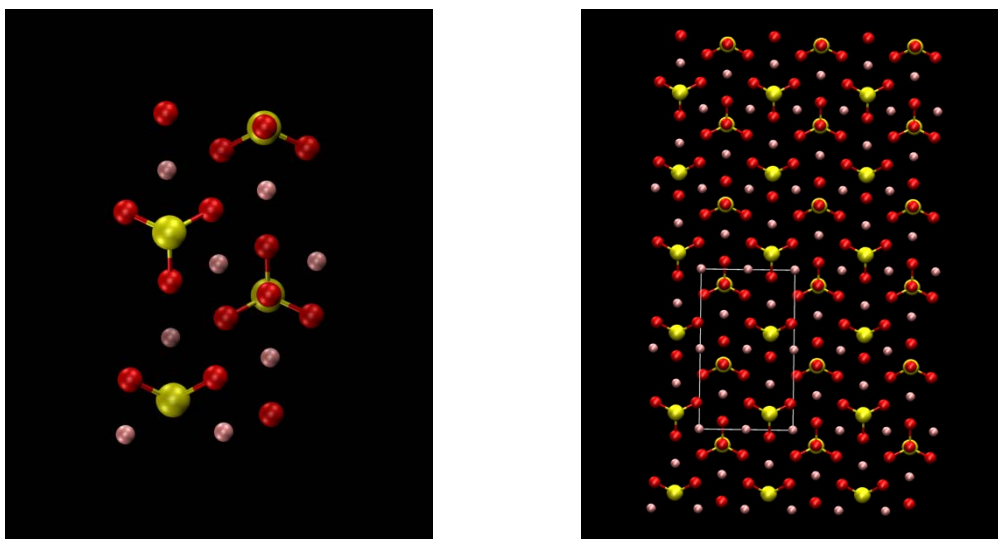
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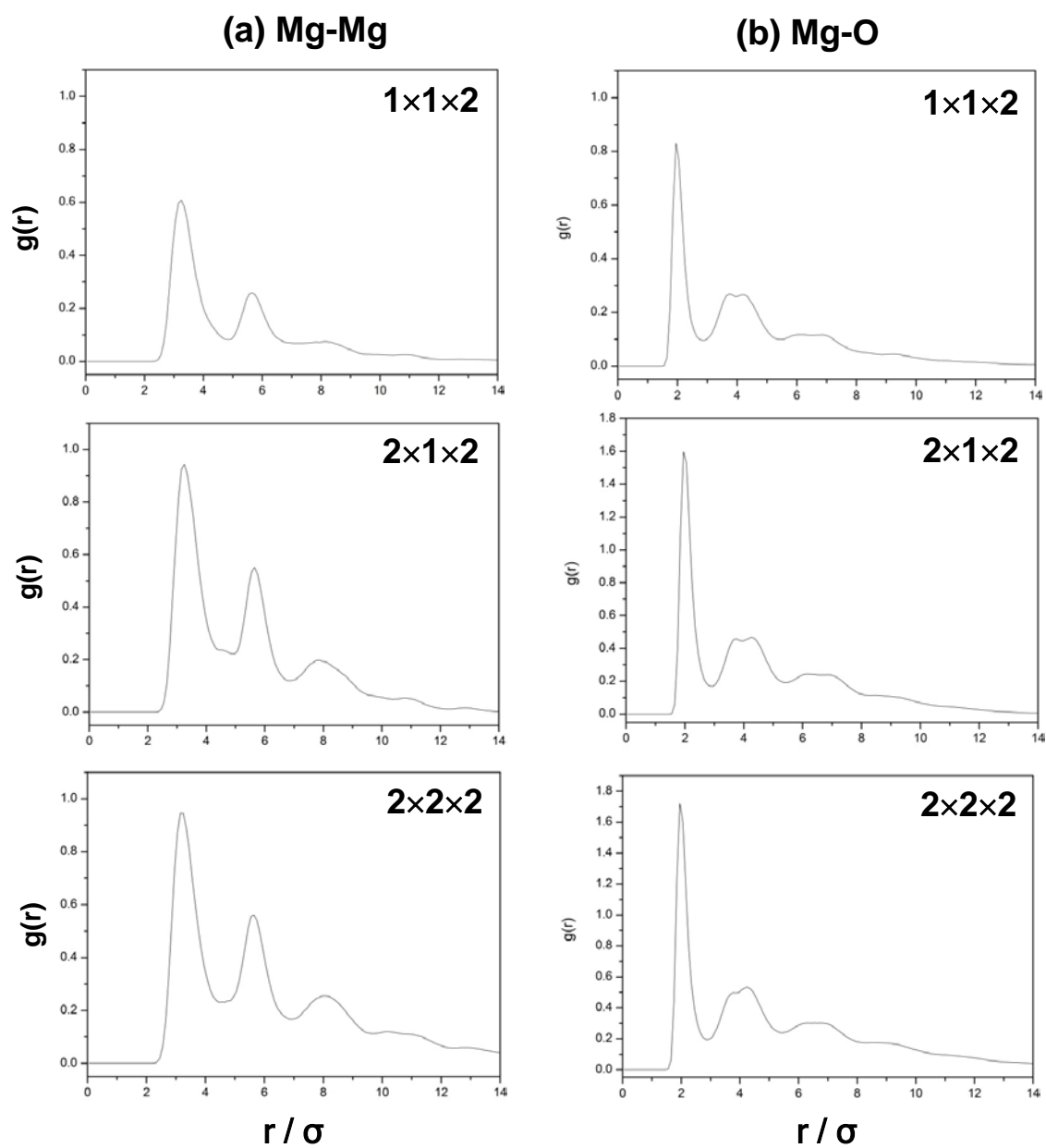
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**Figure S1.** GULP-optimized structure for the bulk of the crystal Mg<sub>2</sub>SiO<sub>4</sub>. View of the unit cell (left), view of the extended periodic system (right)

**Table S1.** Bond distance ranges of the (1×1×1) Mg<sub>2</sub>SiO<sub>4</sub> bulk structures: experimental, GULP-optimized and B3LYP optimized values.

Parameters	Experimental	GULP	B3LYP
Si-O (Å)	1.616-1.649	1.61-1.67	1.628-1.673
Mg1-O	2.069-2.126	2.05-2.15	2.073-2.131
Mg2-O	2.040-2.166	2.01-2.26	2.062-2.223



**Figure S2.** Mg-Mg (a) and Mg-O (b) pair correlation functions derived from the classical MD simulations for the 1x1x2, 2x1x2 and 2x2x2 systems.

## Cell parameters and fractionary coordinates

Amorphous  $1 \times 1 \times 2$   $\text{Mg}_2\text{SiO}_4$  structure.

a=4.93304476000       $\alpha$ =87.441554  
b=9.37079363000       $\beta$ =90.613072  
c=11.93606723000       $\gamma$ =88.598256

12	0.088033963245	0.071404847491	-0.025783798004
12	-0.023814722733	0.301748472438	-0.333035975045
12	0.473861984392	0.495792988074	0.280404977664
12	0.384569679244	-0.437358025828	-0.191627039204
12	0.437838847985	0.455077110139	-0.437571512971
12	-0.002081268047	-0.044678425945	-0.263148562494
12	0.091303279227	-0.114512819647	0.209388284349
12	0.033010380761	-0.004458243938	0.452832521894
12	0.004546685846	0.243279398245	0.196227733413
12	0.386709360423	0.369960484776	0.044446552325
12	0.495302036361	0.148045197659	0.348584327379
12	0.474109828445	0.201356888186	-0.177051653109
12	0.431241533794	-0.282190068864	0.083483126707
12	0.405005901730	-0.216901158402	-0.392879646620
12	0.070641801819	-0.333455448660	0.406633240999
12	-0.048630992965	-0.287918985156	-0.073566220372
14	-0.456992531532	0.075445737893	0.103434226889
14	-0.498697091246	0.107502367173	-0.399197800553
14	-0.033136132237	0.342781091159	0.413643382933
14	-0.063645498613	0.367384153800	-0.088196958255
14	-0.079776129076	-0.432055956585	0.163472860318
14	-0.062431662068	-0.359032876833	-0.332296590138
14	-0.461515731510	-0.193447505037	0.348933389726
14	-0.445182514108	-0.119392912848	-0.151458036929
8	0.133839397184	0.496546080134	-0.322649386510
8	0.114380911747	-0.488198834049	-0.070375068121
8	0.164631015667	0.447250178740	0.174950570940
8	-0.357813591684	-0.144579031624	-0.280231314476
8	-0.168000082991	-0.401573505571	0.290921016603
8	-0.163680576118	-0.067540243039	-0.092058472000
8	0.336211660607	0.257834950709	-0.384017257585
8	-0.145449269708	-0.142011245524	0.343487832427
8	0.005635826397	-0.283621629084	0.090728881016
8	0.246300226491	-0.011489825222	-0.399534030733
8	0.096783307291	-0.270242311284	-0.231485482184
8	-0.267661085174	0.129552586805	-0.296111457330
8	0.491606370706	0.171062113504	-0.012665473377
8	-0.203254840595	0.373288935816	-0.474371910933
8	0.221881387721	0.461112860791	0.414649852784
8	0.010712668052	-0.263297242874	-0.443875389219
8	0.393139685251	0.183073529774	0.188752117185
8	-0.366354936987	-0.478166125302	0.103657065664
8	-0.267581206392	0.323875026960	0.311116820889
8	-0.014430683760	0.273700779709	0.029090259956
8	0.472917955969	-0.291138000797	0.460402675040
8	-0.478026688476	-0.278117367337	-0.082221853187
8	-0.143491864884	0.046978611362	0.147319919495
8	-0.379833400304	-0.408324081084	-0.326798331950

8	0.369352529225	-0.283668126844	0.252013968250
8	0.363270904931	-0.068070637805	0.086418181465
8	-0.376298304045	0.397604224513	-0.132524289194
8	-0.325681403323	0.076396353108	0.489573712254
8	0.126255256760	0.191725828878	0.390497464230
8	0.087536182341	0.261603274225	-0.174199441117
8	0.341357544219	-0.049030183237	0.340229627315
8	0.307690329745	-0.002106125139	-0.158411620105

Amorphous 2×1×2 Mg<sub>2</sub>SiO<sub>4</sub> structure.

a=10.16843999000      α=89.634659  
b=10.17756989000      β=83.909210  
c=11.32973798000      γ=97.083695

12	0.073460850068	-0.493977325015	-0.246394144523
12	-0.135925146351	-0.398740076291	0.111827092155
12	-0.034187419415	0.297895009031	-0.045494235902
12	0.412711638588	-0.303783645109	0.320407541182
12	-0.182372037422	0.056105938736	-0.167613052425
12	0.140723243551	-0.053976326826	-0.301646552408
12	-0.355101059202	-0.229620684904	0.028886945242
12	0.211817118888	-0.400095498556	-0.005022211422
12	0.484758101519	-0.069709678301	0.463237802126
12	-0.336328446534	0.065614169462	-0.397021139924
12	0.211801094404	-0.155040812056	0.419696197893
12	-0.496824930667	-0.414183706234	-0.180363616838
12	-0.485522029003	-0.485966314524	0.074995896003
12	0.208714618074	0.486124706260	0.468839510002
12	0.181727116951	0.076545330968	-0.061863081008
12	0.248795072453	0.324298976875	0.156925151764
12	0.472840562436	0.088650628260	0.021461249437
12	0.312532000891	0.186888661124	0.442429421675
12	-0.033311959130	-0.263693447213	0.391303036198
12	-0.379481921387	0.051168939897	0.262189357342
12	0.455781472610	0.405856309854	-0.357390581600
12	0.335174401835	-0.144844857974	-0.151166862277
12	-0.086703131806	-0.023809170988	0.276335152573
12	-0.101554683130	0.457700562588	0.420754682306
12	-0.016129642691	0.014925971566	-0.475071693554
12	-0.249919031363	0.499453420111	-0.365090021861
12	-0.307127958117	0.394177831434	-0.136195528195
12	-0.298366608270	-0.280729588524	-0.481232495486
12	-0.349394148137	0.270124843836	0.458154998645
12	0.298892106843	0.032380421263	0.253966641327
12	-0.022531506445	-0.311807142651	-0.374652163848
12	-0.194575424933	-0.325747249442	-0.162674711358
14	0.405493415694	-0.193714870492	0.106263692371
14	0.125079602292	-0.122914556018	0.148997286553
14	-0.468640211687	0.284573243264	0.211049119949
14	-0.133592446413	-0.017332915749	0.047049914770
14	0.101287263800	-0.405141179625	0.234769249704
14	-0.467265491869	0.474749213281	0.371856556743
14	0.166378966189	0.222810896569	-0.348638804044
14	-0.169005989323	0.315789283115	0.195215112159
14	0.304144440980	-0.304386954409	-0.381597190985
14	0.473091344676	0.186192969651	-0.198816628647
14	-0.384284894960	-0.162877424234	-0.278451086096
14	-0.314051989880	-0.231502260870	0.292275082255
14	0.270453818453	0.361812782935	-0.093880661057
14	0.048331872387	-0.238146901597	-0.127242564387
14	0.044303080806	0.234659899379	0.330497128647
14	-0.113958354253	0.262850558828	-0.326887027253
8	-0.212973259924	-0.102318287754	-0.050497855654

8	-0.061450282068	-0.424276754129	0.268709459368
8	0.153424531370	-0.345064735946	-0.154528411012
8	0.393290131075	-0.411308969032	-0.330792337296
8	-0.207752068599	0.340563492564	0.334450078895
8	0.154262310592	-0.397587126908	-0.395458669469
8	-0.400237210754	0.455490185122	-0.257119480461
8	0.102488311660	-0.286121241999	0.129956333143
8	0.378310141565	-0.491923826091	0.371014391581
8	0.040863682969	-0.156744721149	-0.476850823652
8	0.485796621210	0.288269381969	0.361105956426
8	-0.470539086858	0.184445387017	-0.338608303541
8	-0.429975197559	0.229386177763	-0.094637455898
8	-0.472335413383	-0.083350315330	0.056106412021
8	0.179602266515	0.493415609938	0.154200514248
8	0.141964517231	-0.099909132498	-0.110831773448
8	-0.191789920576	-0.172564245439	0.372759948609
8	-0.125489524020	0.101735212077	-0.351069263604
8	-0.349356754477	-0.414505731282	-0.052635825116
8	0.124770671172	0.403163261733	-0.119625213971
8	-0.391572438013	-0.355685650743	0.379976397441
8	-0.216281176072	0.012239608829	0.172799871196
8	0.336158626351	0.008111241339	0.413370029953
8	0.287973544200	0.322146974072	-0.427364494009
8	-0.409174821638	0.443398769226	-0.498323681727
8	-0.281368799379	-0.276599087046	-0.303665129419
8	0.469104675343	0.121607127345	0.194406215203
8	0.233625463803	0.000561068117	0.096574658798
8	-0.111446323463	-0.461932322149	-0.255765866159
8	-0.050949129070	0.108212714607	0.391273274570
8	0.220017591509	0.248246455174	0.006921499018
8	-0.369731690197	0.085736380180	0.438678918538
8	-0.257627108924	-0.274590828171	0.162983901980
8	0.317934749053	-0.234308243360	0.000757826297
8	0.381831601425	0.054907811636	-0.131302154374
8	-0.397048904471	0.456219093971	0.230318359067
8	-0.129978136290	0.409415192191	0.073221226787
8	0.435998954392	0.339798964445	0.118787308745
8	-0.021409420046	0.250922541897	0.200137759470
8	0.361844311383	0.496733120111	-0.055757004427
8	0.288729450989	-0.160470011483	-0.318290308968
8	-0.432427533597	-0.137050877673	0.307565191080
8	0.355506528778	-0.247774292086	0.480488394742
8	0.147043302218	-0.356220066640	0.362446418963
8	-0.161965727136	0.272205085052	-0.182778647603
8	0.201106520808	0.203825617674	0.295496224527
8	-0.021540606956	-0.190649801820	-0.243209389433
8	0.363500635482	0.303302830393	-0.204591152834
8	-0.497462258226	-0.226062599769	-0.177896323783
8	0.084385779956	-0.101455910260	0.293387092015
8	0.146130417063	0.132939795110	-0.227923862024
8	0.150065494670	0.100856586949	-0.440833477832
8	0.046785551725	0.325906578020	-0.342845125079
8	-0.142434925855	-0.388499258301	-0.490775399311
8	-0.405744616378	-0.135165183041	-0.419437221964
8	-0.015882140875	-0.083245134643	0.106317633405
8	-0.072137404128	-0.317011029120	-0.039061934258



8	-0.335937385300	-0.014451244617	-0.238140750988
8	-0.314607463479	0.234398625389	0.166129965578
8	-0.061792298288	0.109852639277	-0.034837907705
8	0.319137615755	-0.167416288441	0.232970457398
8	0.060941608204	0.372196786092	0.403908797668
8	0.474378959863	-0.324817887587	0.142449156725
8	-0.195918553017	0.328349786087	-0.423406501955

Amorphous 2×2×2 Mg<sub>2</sub>SiO<sub>4</sub> structure.

a=9.58976422000      α=85.714872  
b=20.57419425000    β=93.367506  
c=11.93781887000    γ=91.743204

12	-0.366764219280	-0.377918300554	0.025564748863
12	0.238206216175	0.221995226492	-0.401543809988
12	-0.013433567011	-0.318347340150	-0.327954181383
12	0.106944543489	0.104852079097	-0.019908418561
12	-0.005139231183	-0.164052806005	0.168114627911
12	-0.239923147384	-0.384194519302	-0.487513299107
12	-0.380846211971	0.315133726243	0.409574531082
12	-0.280421998652	-0.035352411866	0.423347739102
12	0.346979496471	-0.492684099996	0.102628055207
12	0.343163035900	-0.353595324136	-0.315082329188
12	0.086566255360	-0.401305993028	-0.163244723639
12	-0.391655791235	-0.404943126082	0.249229638090
12	-0.139225353645	-0.247573391449	0.388224214179
12	-0.012718639680	0.418891666554	-0.229705397225
12	0.062286303112	0.175834641213	0.345344244712
12	0.426983054391	0.324500102006	0.243313568109
12	-0.178549612762	0.223668410802	-0.438949532896
12	0.255367667208	-0.216177097495	0.370744652007
12	0.093993139980	-0.303406419558	0.220097812121
12	0.251807221250	-0.260690415889	-0.163509194521
12	0.049992871997	-0.161454525102	-0.200174781859
12	0.366243029205	0.187332906784	0.090119970058
12	0.032832494311	0.150109800813	-0.281738867706
12	-0.439475028401	0.245212519293	-0.311080325336
12	0.139640170064	-0.347638099228	0.490971296279
12	-0.001952177635	-0.412300892679	0.109651132554
12	-0.214205230931	0.354524515741	-0.408358714077
12	-0.478911863176	0.285631122694	-0.062310027940
12	-0.188607927055	-0.158318857349	-0.420971227376
12	-0.080217508913	-0.265527379336	-0.061097993865
12	0.432546568761	-0.068431269198	0.229314605457
12	0.420034252572	-0.189158354610	-0.345596754617
12	-0.496104966363	-0.241818862279	0.190273411376
12	-0.291409244453	-0.129858986138	0.185259183516
12	-0.145316414421	-0.031886694552	0.012205494865
12	0.272873426054	0.071940521842	-0.466587820800
12	0.086668666059	0.482483895485	0.274166124779
12	-0.365104281101	-0.279643847973	-0.380632557098
12	-0.228900766514	0.132232125537	0.129968483255
12	-0.019942618135	0.058770610847	0.217981234441
12	0.444688202943	0.375994152200	-0.455215633096
12	-0.496973764856	-0.099316316465	0.023431355635
12	-0.390411157326	-0.084130186698	-0.362079758623
12	0.083558251362	0.008644657723	-0.186847313165
12	0.459973204880	-0.435015243957	-0.484347942575
12	-0.125754370857	0.344808910691	0.000208373828
12	0.270571371215	0.219645293121	-0.138490906161
12	0.304062528595	0.365802252474	0.019693293162
12	-0.395339178431	0.157124699718	0.311100877104

12	-0.439268338816	0.070803994753	-0.445001129162
12	-0.149728910111	0.366443290634	0.292110108559
12	-0.460499795613	-0.458807725222	-0.162948498751
12	-0.177481400101	0.213624320671	-0.125925697454
12	0.081437909300	-0.062149867363	-0.436714475282
12	0.016196135452	-0.457565866254	-0.362247472172
12	0.433381872002	0.450286148993	0.314605402646
12	-0.421241692369	0.005491025692	-0.193801910476
12	-0.447290861968	0.397489809867	-0.222865773232
12	0.387485903802	0.029458874071	-0.004378463748
12	-0.254069681262	0.474250513356	0.402965122533
12	0.105764544109	0.350713097792	0.486724259290
12	0.184342580553	-0.028283215787	0.337462545654
12	0.274037149102	-0.398480868220	0.293970395422
12	-0.170469513887	-0.485842914148	-0.112393016423
14	-0.057127460082	-0.122072282730	0.355172424696
14	0.126432344933	-0.041340005036	0.073051534300
14	-0.007316033605	0.290782531272	-0.288955602153
14	0.288835265811	0.081109752351	0.230589206879
14	-0.206427500005	-0.366034157917	-0.215568034800
14	-0.074811416825	-0.396378098056	0.358270449303
14	0.269232797936	0.493759398761	-0.275675205494
14	-0.450788438467	0.435748328743	0.031176611052
14	-0.254578987570	0.492442371719	0.182688197451
14	0.371730537596	0.186715998905	0.384470652331
14	-0.285891134061	-0.146474180969	-0.116485077595
14	-0.425658237370	0.157368408291	-0.113964729802
14	0.080359122225	0.316001446957	0.217496199173
14	-0.159417392010	0.006766584922	-0.371761796336
14	-0.212292563954	-0.284807696557	0.130061238811
14	-0.346577963105	0.015614752098	0.177627017742
14	0.061386809004	0.476440946081	0.000116839419
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