

Supplementary Material for “Path Integral Monte Carlo and Density Functional Molecular Dynamics Simulations of Warm, Dense MgSiO₃”

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TABLE I: EOS table of MgSiO₃ pressures and internal energies at density-temperature conditions simulated in this work.

Method	T (K)	P (GPa)	P_{σ} (GPa)	E (Ha/MgSiO ₃)	E_{σ} (Ha/MgSiO ₃)
$\rho = 0.320791 \text{ g cm}^{-3}$					
PIMC	1010479	985.7	17.7	-402.925	3.158
PIMC	1347305	1422.3	13.8	-276.376	2.487
PIMC	2020958	2419.0	16.6	6.744	3.003
PIMC	4041916	5461.9	18.4	761.416	3.343
PIMC	8083831	11596.9	19.2	2031.248	3.426
PIMC	16167663	23410.0	20.9	4156.543	3.732
PIMC	32335325	47127.6	27.8	8401.270	4.973
PIMC	64670651	94437.7	38.0	16862.431	6.795
PIMC	129341301	188960.2	48.7	33763.412	8.700
PIMC	517365204	756025.3	77.4	135150.036	13.851
$\rho = 0.801978 \text{ g cm}^{-3}$					
PIMC	1010479	2244.3	51.7	-440.018	3.691
PIMC	1347305	3448.1	43.4	-322.514	3.106
PIMC	2020958	5670.7	53.3	-72.522	3.817
PIMC	4041916	13195.9	60.8	660.024	4.400
PIMC	8083831	28760.1	55.4	1988.394	3.977
PIMC	16167663	58393.2	67.3	4133.516	4.809
PIMC	32335325	117588.7	81.1	8374.153	5.806
PIMC	64670651	235876.9	119.2	16837.664	8.521
PIMC	129341301	471753.6	170.8	33709.072	12.211
$\rho = 1.603955 \text{ g cm}^{-3}$					
PIMC	1010479	4404.2	98.1	-465.104	3.488
PIMC	1347305	6413.6	84.6	-366.495	3.020
PIMC	2020958	11119.7	91.6	-119.815	3.282
PIMC	4041916	26016.8	101.4	590.126	3.690
PIMC	8083831	56864.2	104.1	1933.526	3.735
PIMC	16167663	116284.9	112.8	4100.330	4.030
PIMC	32335325	235230.3	177.3	8364.443	6.346
PIMC	64670651	471003.6	224.4	16801.333	8.029
PIMC	129341301	943488.3	293.6	33700.042	10.498
PIMC	258682602	1889359.3	439.1	67524.645	15.698
PIMC	517365204	3778760.7	499.9	135086.861	17.872
$\rho = 3.207911 \text{ g cm}^{-3}$					
PIMC	1010479	8907.8	188.5	-481.764	3.370
PIMC	1347305	12548.4	162.5	-396.860	2.905
PIMC	2020958	21330.5	176.0	-176.110	3.142
PIMC	4041916	50169.5	209.2	506.925	3.775
PIMC	8083831	112272.2	202.9	1862.233	3.702

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Method	T (K)	P (GPa)	P_σ (GPa)	E (Ha/MgSiO ₃)	E_σ (Ha/MgSiO ₃)
PIMC	16167663	231967.5	227.7	4069.172	4.058
PIMC	32335325	468962.9	302.5	8322.121	5.418
PIMC	64670651	942121.5	410.7	16790.626	7.345
PIMC	129341301	1885785.5	608.2	33667.807	10.886
PIMC	258682602	3777318.6	866.4	67489.822	15.493
$\rho = 6.415822 \text{ g cm}^{-3}$					
DFT-MD	6736	351.4	1.2	-714.235	0.002
DFT-MD	10000	392.9	0.6	-713.996	0.003
DFT-MD	20000	506.1	1.4	-713.280	0.008
DFT-MD	50523	788.0	2.0	-711.160	0.010
DFT-MD	67364	939.8	3.4	-709.826	0.013
DFT-MD	101047	1262.7	3.2	-706.736	0.013
DFT-MD	126309	1527.5	5.3	-704.003	0.023
DFT-MD	202095	2405.8	7.5	-694.333	0.028
DFT-MD	252619	3063.8	7.8	-686.659	0.034
DFT-MD	505239	7022.0	10.8	-639.371	0.045
DFT-MD	673652	10164.3	20.6	-603.052	0.090
DFT-MD	842065	13484.2	21.3	-564.623	0.097
DFT-MD	1010479	17049.2	18.7	-524.482	0.122
PIMC	1347305	23775.1	314.6	-434.797	2.809
PIMC	2020958	41539.5	364.3	-225.127	3.244
PIMC	4041916	97944.7	399.6	428.832	3.633
PIMC	8083831	220211.5	402.4	1763.220	3.664
PIMC	16167663	461535.0	419.4	4018.105	3.723
PIMC	32335325	936225.8	644.3	8286.139	5.755
PIMC	64670651	1882143.3	900.5	16754.661	8.049
PIMC	129341301	3770874.5	1160.5	33647.205	10.370
PIMC	517365204	15115995.9	2234.2	135074.521	19.987
$\rho = 9.623733 \text{ g cm}^{-3}$					
DFT-MD	20000	1406.6	2.3	-712.107	0.008
DFT-MD	50523	1840.5	3.1	-709.905	0.014
DFT-MD	67364	2076.5	2.4	-708.596	0.010
DFT-MD	101047	2558.3	5.3	-705.650	0.016
DFT-MD	126309	2957.3	7.5	-703.124	0.021
DFT-MD	202095	4250.6	8.8	-694.204	0.028
DFT-MD	252619	5188.0	18.8	-687.176	0.046
DFT-MD	505239	11116.8	20.2	-643.237	0.051
DFT-MD	673652	15701.7	24.7	-609.333	0.067
DFT-MD	842065	20740.2	17.8	-572.972	0.098
DFT-MD	1010479	25879.7	37.9	-535.258	0.165
PIMC	1347305	37637.0	486.1	-437.092	2.892
PIMC	2020958	60856.9	546.9	-255.439	3.264
PIMC	4041916	144619.5	618.6	379.405	3.703
PIMC	8083831	326621.6	580.4	1700.569	3.530
PIMC	16167663	688369.7	652.0	3973.287	3.848
PIMC	32335325	1401786.0	896.0	8254.632	5.359
PIMC	64670651	2817248.6	1144.2	16707.029	6.815
PIMC	129341301	5656481.0	1629.2	33637.803	9.716
PIMC	258682602	11326138.5	2520.7	67433.274	15.043
PIMC	517365204	22672033.9	1764.7	135054.478	10.487
$\rho = 12.831643 \text{ g cm}^{-3}$					
DFT-MD	20000	2846.3	2.8	-710.497	0.005
DFT-MD	50523	3450.3	5.0	-708.156	0.018
DFT-MD	67364	3756.7	4.8	-706.880	0.014
DFT-MD	101047	4401.4	9.8	-704.020	0.023
DFT-MD	126309	4898.4	9.4	-701.638	0.025
DFT-MD	202095	6607.8	10.7	-693.218	0.026
DFT-MD	252619	7901.6	18.8	-686.565	0.033

TABLE I – *Continued from previous page*

Method	T (K)	P (GPa)	P_σ (GPa)	E (Ha/MgSiO ₃)	E_σ (Ha/MgSiO ₃)
DFT-MD	505239	15741.3	20.1	-645.044	0.051
DFT-MD	673652	21767.8	33.9	-612.866	0.075
DFT-MD	842065	28294.3	33.1	-578.295	0.143
DFT-MD	1010479	35202.6	40.5	-541.778	0.104
PIMC	1347305	49919.6	632.4	-450.119	2.821
PIMC	2020958	82595.4	743.5	-264.395	3.324
PIMC	4041916	191268.2	811.7	348.530	3.646
PIMC	8083831	431752.7	774.3	1650.585	3.510
PIMC	16167663	916105.5	840.7	3946.426	3.762
PIMC	32335325	1867384.2	1239.0	8235.245	5.533
PIMC	64670651	3758100.5	1368.5	16704.335	6.085
PIMC	129341301	7542418.4	2419.6	33630.976	10.843
PIMC	258682602	15102637.0	4484.4	67430.616	20.067
$\rho = 14.435599 \text{ g cm}^{-3}$					
DFT-MD	50523	4453.6	3.7	-707.214	0.011
DFT-MD	67364	4808.0	5.0	-705.907	0.015
DFT-MD	101047	5494.4	10.7	-703.072	0.024
DFT-MD	126309	6080.9	18.8	-700.760	0.032
DFT-MD	202095	8048.9	14.4	-692.476	0.029
DFT-MD	252619	9451.2	25.4	-686.006	0.035
DFT-MD	505239	18245.1	31.6	-645.524	0.052
DFT-MD	673652	25064.9	42.0	-613.844	0.071
DFT-MD	842065	32353.3	52.8	-579.942	0.106
DFT-MD	1010479	40062.6	38.5	-544.214	0.090
PIMC	1347305	57845.2	715.5	-447.525	2.838
PIMC	2020958	92108.0	835.8	-275.830	3.307
PIMC	4041916	214810.1	932.0	336.524	3.732
PIMC	8083831	483413.8	913.5	1627.865	3.661
PIMC	16167663	1026248.3	858.2	3921.820	3.366
PIMC	32335325	2097429.7	1361.8	8215.810	5.426
PIMC	64670651	4228211.5	1666.0	16701.336	6.614
PIMC	129341301	8479397.1	2594.5	33604.136	10.332
PIMC	258682602	16986835.9	4439.7	67412.875	17.594
PIMC	517365204	34004000.2	2914.1	135028.777	11.535
$\rho = 16.039554 \text{ g cm}^{-3}$					
DFT-MD	50523	5622.7	3.3	-706.143	0.008
DFT-MD	67364	5998.1	6.0	-704.878	0.019
DFT-MD	101047	6700.0	16.8	-702.115	0.020
DFT-MD	126309	7378.3	13.9	-699.830	0.018
DFT-MD	202095	9567.4	23.6	-691.690	0.043
DFT-MD	252619	11112.8	26.5	-685.392	0.057
DFT-MD	505239	20799.2	23.2	-645.857	0.038
DFT-MD	673652	28420.9	32.6	-614.718	0.076
DFT-MD	842065	36466.7	55.0	-581.374	0.094
DFT-MD	1010479	45025.4	29.3	-546.250	0.067
PIMC	1347305	62594.9	792.6	-457.276	2.830
PIMC	2020958	103599.2	907.8	-276.743	3.236
PIMC	4041916	238054.4	1033.9	325.205	3.703
PIMC	8083831	537422.7	1047.1	1616.055	3.809
PIMC	16167663	1140645.8	1096.4	3914.302	3.917
PIMC	32335325	2330647.1	1649.9	8210.748	5.912
PIMC	64670651	4696072.5	1661.2	16689.982	5.925
PIMC	129341301	9420987.0	2670.4	33598.605	9.579
PIMC	258682602	18879584.8	4285.3	67429.068	15.321
PIMC	517365204	37777913.9	3951.9	135010.260	14.170
$\rho = 19.247465 \text{ g cm}^{-3}$					
DFT-MD	50523	8317.4	6.3	-703.943	0.015
DFT-MD	126309	10340.8	25.9	-697.773	0.026

TABLE I – *Continued from previous page*

Method	T (K)	P (GPa)	P_{σ} (GPa)	E (Ha/MgSiO ₃)	E_{σ} (Ha/MgSiO ₃)
DFT-MD	202095	12958.5	25.0	-689.886	0.045
DFT-MD	252619	14884.3	48.1	-683.914	0.066
DFT-MD	505239	26418.2	34.8	-645.984	0.032
DFT-MD	673652	35547.9	58.4	-615.789	0.058
DFT-MD	842065	45193.3	59.4	-583.380	0.084
DFT-MD	1010479	55344.7	64.9	-549.167	0.121
PIMC	1347305	78260.7	966.6	-456.040	2.877
PIMC	2020958	124050.6	1086.0	-286.657	3.236
PIMC	4041916	286047.6	1201.4	308.371	3.589
PIMC	8083831	641458.1	1199.6	1583.582	3.575
PIMC	16167663	1364137.9	1322.6	3885.768	3.955
PIMC	32335325	2794313.6	1778.3	8193.695	5.312
PIMC	64670651	5629957.6	2252.4	16665.926	6.691
PIMC	129341301	11306192.9	3105.8	33595.021	9.251
PIMC	517365204	45335693.3	6332.6	135011.846	18.854
$\rho = 22.455376 \text{ g cm}^{-3}$					
DFT-MD	50523	11640.1	15.8	-702.442	0.905
DFT-MD	67364	11623.9	15.5	-700.474	0.021
DFT-MD	202095	16672.3	54.8	-688.226	0.052
DFT-MD	505239	32713.6	81.2	-645.358	0.087
DFT-MD	673652	43134.8	98.7	-616.334	0.130
DFT-MD	842065	54663.4	181.3	-584.555	0.172
DFT-MD	1010479	66490.5	114.1	-550.946	0.157
PIMC	1347305	92132.5	1069.0	-459.637	2.727
PIMC	2020958	145845.9	1234.3	-292.396	3.143
PIMC	4041916	329924.1	1453.5	285.316	3.723
PIMC	8083831	744158.6	1398.6	1552.599	3.613
PIMC	16167663	1587073.5	1485.2	3862.828	3.829
PIMC	32335325	3255069.8	2203.1	8171.744	5.663
PIMC	64670651	6572269.6	2826.6	16668.890	7.219
PIMC	129341301	13188451.9	4045.4	33583.421	10.298
PIMC	258682602	26424048.2	7386.2	67399.460	18.872
PIMC	517365204	52883432.4	4895.7	134986.763	12.478
$\rho = 25.663287 \text{ g cm}^{-3}$					
DFT-MD	202095	21378.6	93.3	-686.069	0.103
DFT-MD	252619	23905.5	42.8	-680.454	0.038
DFT-MD	505239	39400.4	88.2	-644.716	0.093
DFT-MD	673652	51466.5	165.9	-616.226	0.155
DFT-MD	842065	64514.8	119.4	-585.105	0.116
DFT-MD	1010479	78217.4	307.4	-551.939	0.374
PIMC	1347305	109385.6	1219.4	-456.239	2.724
PIMC	2020958	168477.7	1357.2	-296.396	3.014
PIMC	4041916	374998.9	1691.0	268.237	3.800
PIMC	8083831	844011.8	1649.5	1519.635	3.774
PIMC	16167663	1812658.2	1777.4	3846.798	3.998
PIMC	32335325	3718316.0	2228.3	8159.263	4.977
PIMC	64670651	7504142.3	3179.8	16647.049	7.117
PIMC	129341301	15076258.7	4876.4	33586.921	10.894
PIMC	258682602	30188062.8	7811.0	67370.182	17.443
PIMC	517365204	60440080.8	6705.5	134986.408	14.982
$\rho = 32.079109 \text{ g cm}^{-3}$					
DFT-MD	50523	25027.5	17.0	-693.653	0.021
DFT-MD	202095	32528.5	40.4	-681.020	0.048
DFT-MD	252619	35597.7	123.1	-676.241	0.104
DFT-MD	505239	54803.8	126.0	-642.409	0.103
DFT-MD	673652	69857.1	183.3	-615.052	0.177
DFT-MD	842065	85887.3	165.5	-585.276	0.150
DFT-MD	1010479	103145.5	161.3	-553.188	0.146

TABLE I – *Continued from previous page*

Method	T (K)	P (GPa)	P_{σ} (GPa)	E (Ha/MgSiO ₃)	E_{σ} (Ha/MgSiO ₃)
PIMC	1347305	142611.4	1516.3	-455.777	2.714
PIMC	2020958	212247.3	1705.1	-305.990	3.054
PIMC	4041916	464232.6	2058.3	238.554	3.664
PIMC	8083831	1050564.1	2089.8	1482.573	3.764
PIMC	16167663	2257206.7	2110.7	3810.319	3.782
PIMC	32335325	4643572.5	2981.4	8136.413	5.319
PIMC	64670651	9381000.7	4347.0	16636.045	7.753
PIMC	258682602	37727123.0	8793.7	67347.886	15.693
PIMC	517365204	75542345.3	9190.4	134964.937	16.394
$\rho = 38.494931 \text{ g cm}^{-3}$					
PIMC	1347305	177917.0	1792.2	-452.468	2.671
PIMC	2020958	261470.8	2153.0	-307.051	3.206
PIMC	4041916	564948.4	2468.9	232.916	3.680
PIMC	8083831	1251954.7	2622.0	1444.333	3.954
PIMC	16167663	2698409.7	2534.2	3774.151	3.818
PIMC	32335325	5564785.3	3665.6	8111.753	5.478
PIMC	64670651	11250753.3	5107.8	16616.063	7.637
PIMC	129341301	22607709.2	6297.5	33557.641	9.482
PIMC	258682602	45275049.3	11563.2	67343.882	17.276
PIMC	517365204	90647953.9	11079.4	134953.867	16.539
$\rho = 48.118663 \text{ g cm}^{-3}$					
PIMC	1010479	178573.5	2943.5	-508.641	3.504
PIMC	1347305	224863.8	2362.7	-460.024	2.814
PIMC	2020958	335084.0	2544.9	-309.327	3.023
PIMC	4041916	709416.8	3146.6	216.048	3.750
PIMC	8083831	1567386.7	3056.9	1416.314	3.664
PIMC	16167663	3362881.8	3212.4	3737.250	3.843
PIMC	32335325	6937034.0	4455.2	8070.513	5.311
PIMC	64670651	14048306.5	5242.8	16583.868	6.258
PIMC	129341301	28242489.3	8749.6	33526.000	10.408
PIMC	258682602	56584658.8	16093.2	67323.300	19.145
PIMC	517365204	113320131.2	8826.0	134957.670	10.551
$\rho = 64.158218 \text{ g cm}^{-3}$					
PIMC	1010479	276062.2	2825.5	-490.544	2.527
PIMC	1347305	335299.0	2282.7	-440.517	2.044
PIMC	2020958	469199.9	3002.5	-307.446	2.687
PIMC	4041916	956126.3	3463.2	197.432	3.120
PIMC	8083831	2079234.3	3322.2	1364.268	2.992
PIMC	16167663	4473887.5	3896.9	3691.664	3.494
PIMC	32335325	9243342.9	5485.9	8039.606	4.895
PIMC	64670651	18725696.8	7008.9	16558.398	6.242
PIMC	129341301	37619123.9	9278.1	33475.397	8.241
PIMC	258682602	75456530.9	13092.6	67317.973	11.723
PIMC	517365204	151047161.2	12265.3	134903.290	11.052