Supplementary information for Verma and Karki

S1: Pressure-volume-temperature (*P-V-T*) results calculated from the first-principles molecular dynamics simulations of diopside liquid. Table shows the calculated pressures (GPa) at different volume-temperature conditions shown.

V (cc/mol)	V/Vx	2200 K	2500 K	3000 K	3500 K	4000 K	5000 K	6000 K
				Pressure (P)				
131.7	1.61							1.3
124.4	1.52						0.8	
108.8	1.33					0.3		
103.1	1.26				0.2			
94.9	1.16			0.3				
89.7	1.10	-0.2	0.0					
81.8	1.00		2.3	2.9		4.7		9.5
73.6	0.90		5.6	6.3		8.6		14.9
65.4	0.80		11.9	12.7		16.8		24.7
57.3	0.70			27.2		31.7		43.0
53.2	0.65			37.1		44.2		57.7
49.1	0.60			51.8		61.0		76.5
45.0	0.55					88.3		106.0
40.9	0.50							149.8

S2: Self-diffusivities results (10^{-9} m^2/s) calculated from the first-principles molecular dynamics simulations of diopside liquid at different volume-temperature conditions shown. The results are presented in appropriate significant figures.

V (cc/mol)	V/Vx	2200 K	2500 K	3000 K	3500 K	4000 K	5000 K	6000 K
				Ca Self Diffusivity				
131.7	1.61							89
124.4	1.52						43	
108.8	1.33					19		
103.1	1.26				16			
94.9	1.16			6.7				
89.7	1.10	2.1	3.1					
81.8	1.00		2.4	5.1		11		38
73.6	0.90		1.4	3.9		9.2		21
65.4	0.80		0.72	1.9		7.2		18
57.3	0.70			0.81		3.9		13
53.2	0.65			0.33		2.2		13
49.1	0.60					1.4		8.2
45.0	0.55					0.58		5.3
40.9	0.50							3.5

V (cc/mol)	V/Vx	2200 K	2500 K	3000 K	3500 K	4000 K	5000 K	6000 K
				Mg Self Diffusivity				
131.7	1.61							85
124.4	1.52						39	
108.8	1.33					19		
103.1	1.26				12			
94.9	1.16			6.5				
89.7	1.10	1.5	2.6					
81.8	1.00		2.3	6.4		16		38
73.6	0.90		1.5	5.5		10		25
65.4	0.80		1.05	3.0		9.4		28
57.3	0.70			1.4		4.3		13
53.2	0.65			0.52		3.5		11
49.1	0.60					1.7		10
45.0	0.55					0.62		6.1
40.9	0.50							4.3

V (cc/mol)	V/Vx	2200 K	2500 K	3000 K	3500 K	4000 K	5000 K	6000 K
				Si Self Diffusivity				
131.7	1.61							68
124.4	1.52						31	
108.8	1.33					12		
103.1	1.26				5.5			
94.9	1.16			2.6				
89.7	1.10	0.28	0.53					
81.8	1.00		0.82	2.1		6.9		26
73.6	0.90		0.75	2.3		6.4		25
65.4	0.80		0.58	1.9		6.9		20
57.3	0.70			0.78		3.3		11
53.2	0.65			0.33		2.5		9.3
49.1	0.60					1.2		7.9
45.0	0.55					0.41		5.8
40.9	0.50							4.1

V (cc/mol)	V/Vx	2200 K	2500 K	3000 K	3500 K	4000 K	5000 K	6000 K
			O Self Diffusivity					
131.7	1.61							69
124.4	1.52						37	
108.8	1.33					14		
103.1	1.26				7.5			
94.9	1.16			2.9				
89.7	1.10	0.45	**0.85**					
81.8	1.00		**1.2**	2.7		12		43
73.6	0.90		**1.1**	3.5		10		33
65.4	0.80		**0.99**	2.8		8.1		29
57.3	0.70			1.4		5.6		20
53.2	0.65			0.75		3.3		15
49.1	0.60					2.0		11
45.0	0.55					0.72		8.0
40.9	0.50							5.2

S3: Viscosity results (Pa s) calculated from the first-principles molecular dynamics simulations of diopside liquid at different volume-temperature conditions shown. The results are presented in appropriate significant figures.

V (cc/mol)	V/Vx	2200 K	2500 K	3000 K	3500 K	4000 K	5000 K	6000 K
			Viscosity					
131.7	1.61							0.00041
124.4	1.52						0.00055	
108.8	1.33					0.0017		
103.1	1.26				0.0025			
94.9	1.16			0.0072				
89.7	1.10	0.053	0.022					
81.8	1.00		0.027	0.0085		0.0031		0.0011
73.6	0.90		0.026	0.0065		0.0043		0.0015
65.4	0.80		0.058	0.0090		0.0052		0.0021
57.3	0.70			0.0320		0.0104		0.0035
53.2	0.65			0.1600		0.0183		0.0045
49.1	0.60					0.0380		0.0072
45.0	0.55							0.0105
40.9	0.50							0.0220

S4: Sample INCAR file used in the simulations (3000 K and V_X)

SYSTEM = Diopside Liquid (CaMgSi2O6)

 Startparameter for this Run:
  NWRITE =   2; LPETIM=F   write-flag & timer
  ISTART =   0   job : 0-new 1-cont 2-samecut
  LWAVE = .FALSE.
  LCHARG = .FALSE.

 Electronic Relaxation 1
  ENCUT = 400.00 EV
  NELM   = 20;
  EDIFF = 1E-04   stopping-criterion for ELM
  MAXMIX = 50

 Ionic Relaxation
  NSW   =   100000 number of steps for IOM
  NBLOCK =   1; KBLOCK =   1   inner block; outer block
  ISYM =   0
  ISIF =   2

  POTIM = 1.00   time-step for ion-motion
  TEBEG = 3000 ; TEEND=3000 initial temperature
  SMASS = 0.00   Nose mass-parameter (am)
  NPACO = 104
  APACO = 10.4

 DOS related values:
  ISMEAR =   -1; SIGMA = .2585 broadening in eV -4-tet -1-fermi 0-gaus

 Electronic Relaxation 2
  IALGO =   48   algorithm
  LREAL =   A

S5: Sample POSCAR file using supercell of length of 12.953 Ansgtrom and with 160 atoms used in the simulations (at 3000 K and V$_X$)

```
Diopside Liquid (CaMgSi2O6)
 1.000000
  12.9530000000000000    0.0000000000000000    0.0000000000000000
   0.0000000000000000   12.9530000000000000    0.0000000000000000
   0.0000000000000000    0.0000000000000000   12.9530000000000000
  16  16  32  96
Direct
 0.48371132 0.17873153 0.89823302
 0.20562463 0.81285585 0.20453290
 0.63727938 0.60821753 0.41498882
 0.05906639 0.19001347 0.78370497
 0.95095297 0.90132948 0.93199945
 0.79319956 0.14588981 0.74120244
 0.02435480 0.23912880 0.10765790
 0.55249367 0.62317805 0.85023268
 0.03413093 0.55706328 0.05711208
 0.43042644 0.39748710 0.01431805
 0.89599741 0.57994643 0.57594304
 0.86890239 0.12820119 0.22577495
 0.27894783 0.13267027 0.06462266
 0.39175416 0.72729924 0.33237274
 0.00152247 0.83611594 0.38645858
 0.42113014 0.43390378 0.46803076
 0.77858899 0.36747798 0.66988627
 0.58355700 0.79744726 0.65347809
 0.57730558 0.05011265 0.37164815
 0.50145563 0.02851659 0.69210742
 0.24427284 0.94349142 0.55063027
 0.13825535 0.15832576 0.32729905
 0.31150334 0.57553174 0.79284449
 0.28838545 0.96814615 0.89824358
 0.12692349 0.38126674 0.62942178
 0.52487647 0.19160513 0.18898548
 0.14495116 0.70138952 0.57018571
 0.96287581 0.32907092 0.44154435
 0.81691108 0.76416088 0.07699011
 0.84530019 0.02348971 0.46595769
 0.33284152 0.61595284 0.56515230
 0.45978571 0.16507519 0.45800329
 0.00434397 0.96447607 0.13461318
 0.01353330 0.11378898 0.53740410
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0.81090452  0.38536245  0.29295120
0.75411488  0.76494721  0.81909123
0.66413522  0.97368170  0.56200209
0.18802841  0.31972067  0.95216565
0.58925540  0.26041031  0.62648022
0.91584543  0.36241607  0.85289459
0.32534260  0.00891013  0.32989772
0.27987489  0.53083606  0.22190942
0.24929893  0.18314711  0.55072295
0.62717065  0.94569097  0.15949377
0.46323673  0.44256323  0.74287185
0.10052538  0.40723253  0.24601965
0.14452508  0.76246496  0.93876369
0.59960265  0.31974309  0.40182117
0.36452964  0.78336840  0.69663554
0.65315332  0.58142236  0.66529608
0.11760166  0.47044763  0.87843168
0.08756490  0.53118850  0.44888787
0.31071872  0.17277879  0.74594351
0.04345227  0.93194607  0.62607645
0.30769040  0.66783633  0.03561299
0.62048279  0.93470341  0.89588144
0.00075080  0.76048811  0.75585263
0.44196311  0.89092878  0.05727221
0.65130166  0.73510155  0.26242164
0.79680948  0.79411053  0.43825416
0.89261663  0.11567976  0.95060221
0.56046149  0.15598104  0.57556921
0.23926847  0.63369795  0.26374262
0.53302139  0.49572735  0.17007895
0.22840972  0.27424117  0.72841446
0.51016004  0.87604913  0.94680082
0.51210266  0.89135627  0.15358091
0.68113693  0.01126851  0.44292114
0.19443751  0.44578948  0.97722193
0.54556460  0.54449031  0.68982270
0.54648381  0.93428485  0.59121300
0.77036663  0.48699842  0.22459560
0.83787747  0.11967174  0.07392870
0.37284200  0.64913114  0.92074529
0.82476639  0.36456398  0.92709764
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0.08121044 0.89192096 0.20878744
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0.99095178 0.88036938 0.72408239
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0.60276943 0.03846545 0.82993604
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0.12942166 0.40568032 0.78045387
0.24524940 0.08388903 0.79435598
0.43871550 0.04858908 0.33763193
0.02162308 0.45937644 0.52236908
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0.79226417 0.77868230 0.94271611
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