Supporting Information for

Study of high-pressure thermophysical properties for orthocarbonate Sr_3CO_5 using deep learning molecular dynamics simulations

Xin-Xuan Wang[a], Ting Song[a,*], Zhen-Shuai Lei[b], Xiao-Wei Sun[a], Jun-Hong Tian[a], Zi-Jiang Liu[a]

[a] *School of Mathematics and Physics, Lanzhou Jiaotong University, Lanzhou 730070, China*

[b] *Faculty of Science, Wuhan University of Technology, Wuhan 430079, China*

This supporting information lists the validation data for the calculation of elastic constants using the Deep Learning Potential Function model described in the main text, as well as the variation of elastic modulus, density and wave velocity as a function of temperature using the DP model.

* Corresponding author.
E-mail: songting_lzjtu@yeah.net

Table S1 The C_{ij} (GPa), B (GPa), G (GPa), ρ (g/cm^3), V_P (km/s) and V_S (km/s) of Sr_3CO_5-*Cmcm* and Sr_3CO_5-*I4/mcm* obtained via DPMD simulations at 0 K and compared with DFT calculation results (in parentheses).

	Sr_3CO_5-*Cmcm*		Sr_3CO_5-*I4/mcm*		
	10 GPa	30 GPa	30 GPa	80 GPa	120 GPa
C_{11}	213.1 (224.0)	361.5 (361.7)	323.5 (321.0)	560.4 (561.9)	747.1 (741.8)
C_{12}	66.5 (71.6)	144.6 (126.1)	146.5 (150.0)	271.2 (287.2)	380.9 (396.1)
C_{13}	88.9 (93.5)	158.8 (141.9)	184.3 (176.0)	342.1 (336.0)	463.8 (459.4)
C_{22}	219.7 (221.3)	375.1 (339.4)	-	-	-
C_{23}	105.7 (107.1)	207.1 (186.6)	-	-	-
C_{33}	266.5 (269.6)	418.5 (398.2)	354.3 (351.1)	569.4 (574.7)	720.5 (736.3)
C_{44}	78.3 (86.1)	110.2 (121.2)	119.6 (128.1)	202.1 (205.7)	239.0 (259.1)
C_{55}	79.0 (77.4)	93.8 (90.4)	-	-	-
C_{66}	44.7 (48.9)	66.8 (63.6)	108.4 (105.3)	169.5 (163.9)	206.4 (203.7)
B	135.7 (138.5)	240.0 (221.8)	224.7 (221.2)	398.9 (401.2)	536.4 (538.4)
G	67.9 (70.5)	95.1 (95.1)	99.4 (102.8)	158.2 (159.6)	190.9 (197.8)
ρ	5.3 (5.3)	5.9 (5.9)	6.0 (6.0)	7.1 (7.1)	7.7 (7.7)
V_P	6.5 (6.6)	7.8 (7.7)	7.7 (7.7)	9.3 (9.3)	10.1 (10.1)
V_s	3.6 (3.6)	4.0 (4.0)	4.1 (4.1)	4.7 (4.7)	5.0 (5.0)

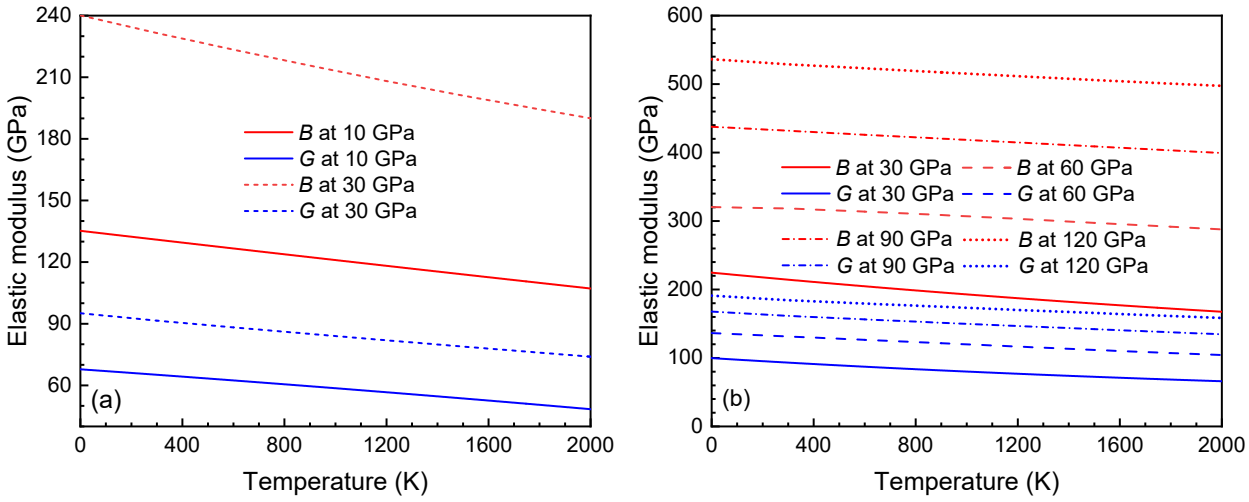

Fig. S1 The elastic moduli of (a) Sr_3CO_5-*Cmcm* and (b) Sr_3CO_5-*I4/mcm* as a function of temperature obtained from DPMD simulations.

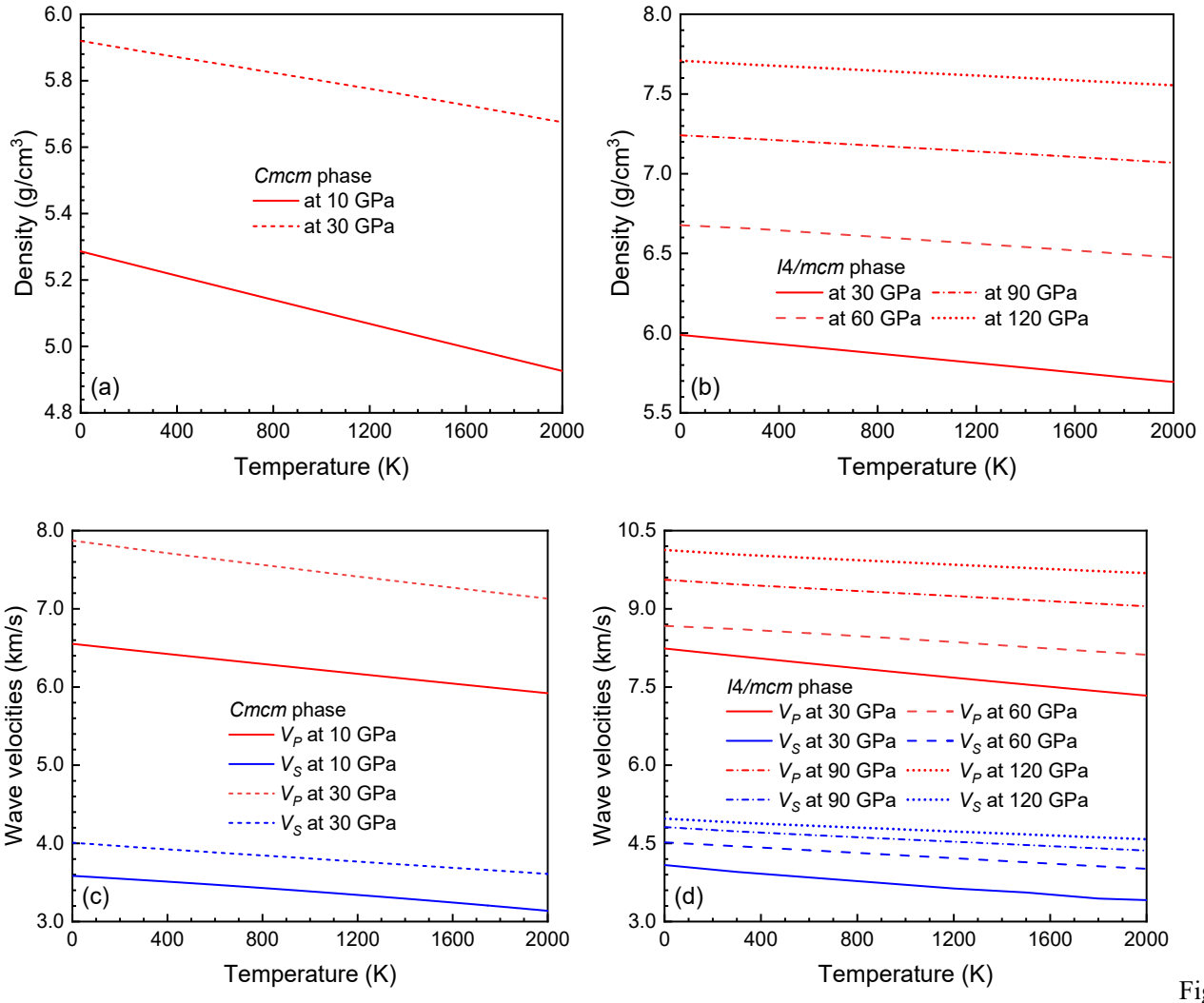

Fig. S2 Temperature dependence of density and sound velocities for Sr_3CO_5-*Cmcm* and Sr_3CO_5-*I4/mcm* obtained by DPMD simulations, with (a) and (c) representing the *Cmcm* phase, (b) and (d) representing the *I4/mcm* phase.