Supplementary Material for: Metastability and Ostwald Step Rule in the Crystallisation of Diamond and Graphite from Molten Carbon

Davide Donadio,[1] Margaret L. Berrens,[1,2] Wanyu Zhao,[3] Shunda Chen,[3] and Tianshu Li[3]

[1)]*Department of Chemistry, University of California Davis*[a)]

[2)]*Quantum Simulations Group, Physics Division, Lawrence Livermore National Laboratory, Livermore, California 94550, United States.*

[3)]*Department of Civil and Environmental Engineering, George Washington University*

[a)]Electronic mail: ddonadio@ucdavis.edu.

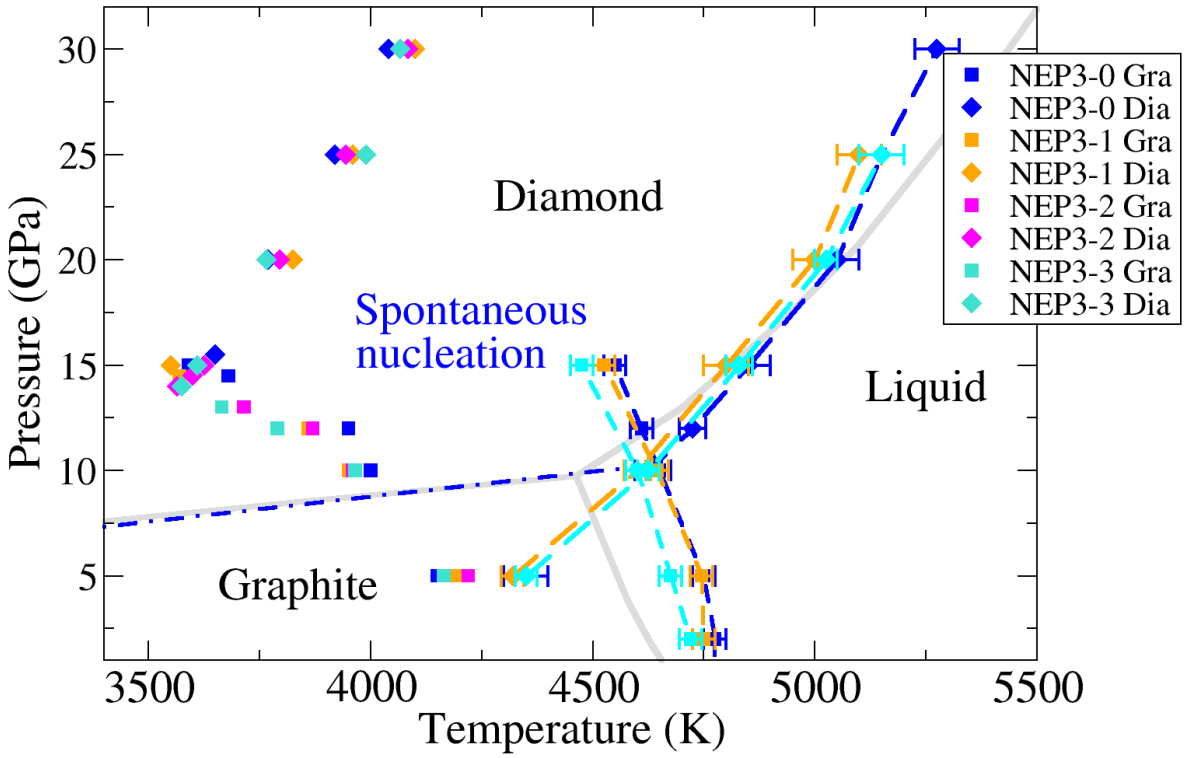

FIG. S1. Phase diagram and spontaneous crystallisation temperature with four different parameterizations of the NEP machine learning potential.

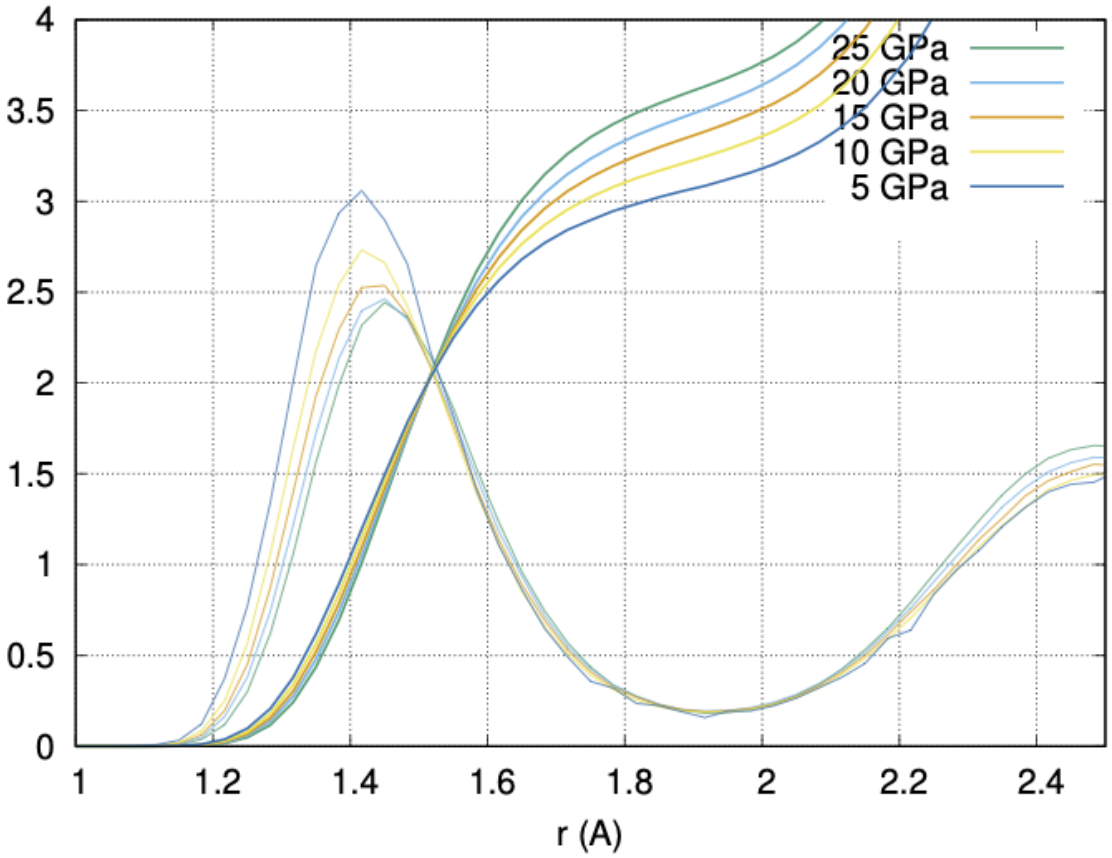

FIG. S2. Radial distribution function (a) and angular distribution function (b) of liquid carbon at 4000 K and different pressures.

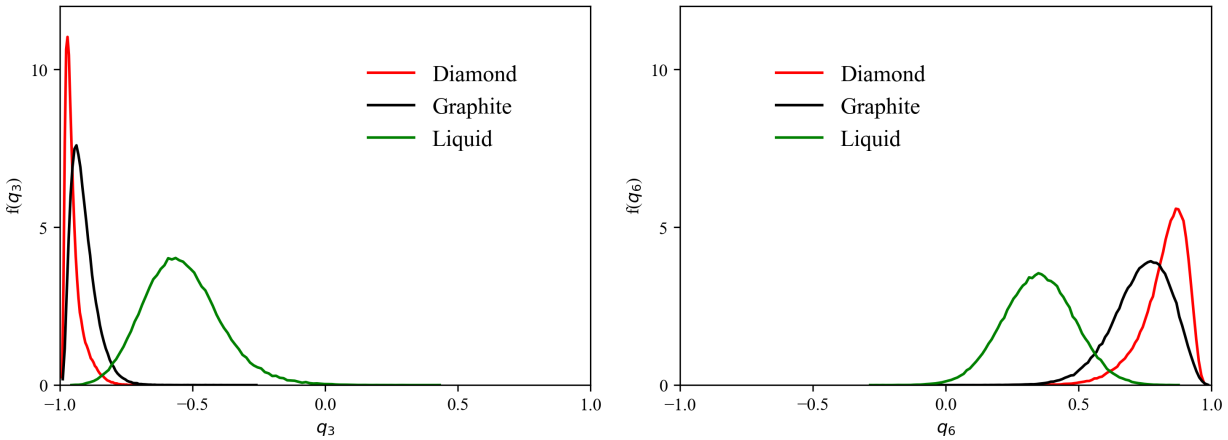

FIG. S3. Distribution of local bond-order parameter (a) q_3 and (b) q_6 for diamond, graphite, and liquid carbon at 4000 K and 15 GPa.

TABLE I. Structural and elastic properties of graphite and diamond. The elastic constants of diamond were measured by resonant-ultrasound spectroscopy and those of graphite by inelastic X-ray scattering.[1,2]

Diamond	NEP	LDA[3]	Experiments[1]
a (Å)	3.54	3.55	3.61
ω_{LO} (THz)	39.1	x	39.9
C_{11} (GPa)	1116	1106	1079
C_{12} (GPa)	144	149	127
C_{44} (GPa)	594	593	578

Graphite	NEP	LDA[4]	Experiments[2]
a (Å)	2.44	2.44	2.46
c (Å)	6.60	6.63	6.71
ω_{LO} (THz)	42.8	47.7	47.4
C_{11} (GPa)	1128	1118	1109
C_{12} (GPa)	179	235	139
C_{33} (GPa)	36.0	29.5	38.7
C_{44} (GPa)	7.04	4.5	4.95

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