

Supplementary Information

Table 1 Zero temperature phase diagram of the optimized potential for the diamond target structure. We show the stable phase (column 1), its lattice parameters (column 2), the corresponding stable pressure range (column 3) and the stable density range (column 4). The parameter nomenclature is the same as described in Ref¹.

Lattice acronyms: face-centered cubic (FCC), body-centered cubic (BCC), diamond (DIA), simple cubic (SC), wurtzite (WUR), hexagonal (SH), body centred orthorhombic (BCO), rhombohedral (hR).

Lattice	Parameters	Pressure ($P\sigma^3/\epsilon$)	Density ($\rho\sigma^3$)
hR	1.417	0.1 - 2.0	0.27547 - 0.59252
BCC		2.1 - 3.6	0.60570 - 0.73819
hR	0.2162	3.7 - 3.9	0.84149 - 0.85735
BCO	0.6234, 1.7403	4.0 - 4.4	0.87317 - 0.90280
SH	0.61	4.5 - 6.4	0.91409 - 1.03991
A7	3.8874, 0.3172	6.5 - 7.9	1.08248 - 1.16240
DIA		8.0 - 14.5	1.21318 - 1.52094
SH	1.4124	14.6 - 15.3	1.62509 - 1.65489
SH	1.4148	15.4 - 15.9	1.65918 - 1.67987
SH	1.4157	16.0 - 16.4	1.68398 - 1.70019
SH	1.4171	16.5 - 17.9	1.70425 - 1.75908
A20	1.6658, 0.5892, 0.1745	18.0 - 18.3	1.82194 - 1.83304
A20	1.7447, 0.6455, 0.3331	18.4 - 26.9	1.83805 - 2.13483

Table 2 Zero temperature phase diagram of the optimized potential for the simple cubic target structure. We show the stable phase (column 1), its lattice parameters (column 2), the corresponding stable pressure range (column 3) and the stable density range (column 4). The parameter nomenclature is the same as described in Ref¹.

Lattice	Parameters	Pressure ($P\sigma^3/\epsilon$)	Density ($\rho\sigma^3$)
hR	1.417	1.1 - 3.4	0.54192 - 0.74723
BCC		3.5 - 7.4	0.76007 - 1.0179
hR	0.3025	7.5	1.03577
BCO	2.006, 1.0248	7.6 - 7.9	1.05841 - 1.07616
BCO	0.9667, 1.9956	8.0 - 8.2	1.08617 - 1.09760
β Sn	0.6527	8.3 - 11.1	1.12945 - 1.26788
SC		11.2 - 16.9	1.30781 - 1.53378
β Sn	3.5155	17.0 - 17.3	1.57197 - 1.58322
β Sn	3.4898	17.4 - 18.2	1.58746 - 1.61659
β Sn	3.4774	18.3 - 19.2	1.62039 - 1.65191
β Sn	3.4551	19.3 - 21.4	1.65563 - 1.72502
β Sn	3.4385	21.5 - 25.4	1.72837 - 1.84539
A20	2.9956, 0.9897, 0.8671	25.5 - 26.0	1.8949 - 1.909750
FCC		26.1 - 29.9	1.95247 - 2.06796

References

- [1] S. Prestipino, F. Saija and G. Malescio, *Soft Matter*, 2009, **5**, 2795.