Supplementary Information for ”Nucleation mechanism for the direct graphite-to-diamond phase transition”

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A. Rhombohedral graphite to cubic diamond

B. Orthorhombic graphite to hexagonal diamond

C. AA graphite to hexagonal diamond

Figure 1: Representative structures along high-symmetry concerted transformation paths from graphite to diamond. Zero-temperature structures and configurations with displaced atoms in the 0–100 GPa range were included in the neural network training set.
Figure 2: Representative structures of the interface between rhombohedral graphite and cubic diamond. Zero-temperature structures and configurations with displaced atoms in the 0–80 GPa range were included in the neural network training set. A. (100)$_G$ interface. B. (120)$_G$ interface. C. (001)$_G$ interface. D. Bent graphite layers present in the vicinity of the (001)$_G$ interface with different degrees of distortion. Structures of similar interfaces between orthorhombic graphite and hexagonal diamond were also included in the training set.