SACADA Database Code: 480

Topology: 4^{12}T7

# of independent nodes (IN): 12
Transitivity: [(12)(24)(23)(11)]
Space Group: P1
Pearson: aP12
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{12}T7 (SACADA #480)		3.254		1.481	313.1	310.5	55.5	SACADA[1]
G188								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8117.2072	1187.7373	795.4352	-447.0285	-69.3425	-173.3388
1187.7373	7638.6510	1041.0965	-498.4230	50.5282	-86.1138
795.4352	1041.0965	6531.8566	-294.2774	213.7030	114.7656
-447.0285	-498.4230	-294.2774	3704.2709	91.5335	39.5709
-69.3425	50.5282	213.7030	91.5335	2637.2584	-518.0788
-173.3388	-86.1138	114.7656	39.5709	-518.0788	2898.6611

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].