SACADA Database Code: 326

Topology: 4^{12}T3

# of independent nodes (IN): 12
Transitivity: [(12)(19)(19)(11)]
Space Group: C2/m
Pearson: mS48
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{12}T3 (SACADA #326)		3.491		0.641	418.4	481.2	90.7	SACADA[1]
24A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

9945.6981	1076.4246	1467.0940	0.0000	0.0000	-90.3303
1076.4246	11205.0347	378.4903	0.0000	0.0000	130.5836
1467.0940	378.4903	10659.2643	-0.0000	-0.0000	-157.5525
0.0000	0.0000	-0.0000	5189.4199	66.0556	-0.0000
0.0000	0.0000	-0.0000	66.0556	4371.7105	-0.0000
-90.3303	130.5836	-157.5525	-0.0000	-0.0000	4960.8179

[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].