SACADA Database Code: 243

Topology: 4^5T11

# of independent nodes (IN): 5
Transitivity: [5886]
Space Group: Pmmn
Pearson: oP16
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^5T11 (SACADA #243)		3.411		0.737	395.8	445.6	83.6	SACADA[1]
Z-ACA		3.353	2.261		375.97		78.74	doi: 10.1039/c2cp40531h
Z-ACA								doi: 10.3103/s1063457612060123

Elasticity tensor (kBar)[1]

8116.5011	330.7403	1240.7887	0.0000	-0.0000	0.0000
330.7403	11451.7400	1166.2141	-0.0000	0.0000	-0.0000
1240.7887	1166.2141	11083.9375	-0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	3765.4075	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	5293.5985	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	4183.6050

[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].