SACADA Database Code: 256

Topology: 4^6T15

# of independent nodes (IN): 6
Transitivity: [6985]
Space Group: Pmn21
Pearson: oP12
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
4^6T15 (SACADA #256)		3.444		0.677	427.0	477.6	89.4	SACADA[1]
12D	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11386.1708	501.5001	1025.5845	-0.0000	-0.0000	-0.0000
501.5001	10236.6473	1256.1833	-0.0000	-0.0000	0.0000
1025.5845	1256.1833	11314.5131	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	4023.9125	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	4601.8107	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	5338.5796

[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].