SACADA Database Code: 351

Topology: 4^{24}T1

# of independent nodes (IN): 24
Transitivity: [(24)(36)(34)(22)]
Space Group: Pm
Pearson: mP24
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^{24}T1 (SACADA #351)		3.491		0.657	418.0	487.0	92.0	SACADA[1]
24B	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10723.8999	382.3349	950.4000	0.0000	-0.0000	-368.2240
382.3349	11294.0771	968.4283	-0.0000	0.0000	40.3582
950.4000	968.4283	11017.3194	-0.0000	0.0000	295.4403
0.0000	-0.0000	-0.0000	4187.9209	59.0442	0.0000
-0.0000	0.0000	0.0000	59.0442	5246.4648	0.0000
-368.2240	40.3582	295.4403	0.0000	0.0000	4765.0814

[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].