SACADA Database Code: 337

Topology: 4^{16}T2

# of independent nodes (IN): 16
Transitivity: [(16)(24)(22)(14)]
Space Group: Cm
Pearson: mS32
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^{16}T2 (SACADA #337)		3.463		0.664	413.4	475.8	89.7	SACADA[1]
16B	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10367.0832	479.8766	874.6426	-0.0000	-0.0000	65.3202
479.8766	11113.8077	940.0228	-0.0000	0.0000	-167.9571
874.6426	940.0228	11173.2882	-0.0000	0.0000	3.7698
-0.0000	-0.0000	-0.0000	4137.3807	-194.7858	-0.0000
-0.0000	0.0000	0.0000	-194.7858	5159.9484	0.0000
65.3202	-167.9571	3.7698	-0.0000	0.0000	4468.1347

[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].