SACADA Database Code: 176

Topology: pbz-m

# of independent nodes (IN): 3
Transitivity: [3563]
Space Group: Pn-3m
Pearson: cP96
Coordination Number (CN): 3

Year: 1991

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pbz-m (SACADA #176)		1.198		0.766	140.7	68.7	9.0	SACADA[1]
D8								doi: 10.1038/352762a0
D8								doi: 10.1016/0008-6223(92)90066-6
D8								doi: 10.1098/rsta.1993.0045
D8								doi: 10.1016/0009-2614(93)85009-d
D8								link
D8		1.21			148			doi: 10.1016/0956-7151(94)90210-0
D8								link
D8								doi: 10.1016/s0960-8974(97)00003-x
D8								doi: 10.1088/1367-2630/5/1/126
D8			0.2		179	75.5		doi: 10.1088/1367-2630/5/1/123

Elasticity tensor (kBar)[1]

2336.4978	941.6646	941.6646	-0.0001	-0.0000	-0.0001
941.6646	2336.4978	941.6646	-0.0001	-0.0001	-0.0000
941.6646	941.6646	2336.4978	-0.0000	-0.0001	-0.0001
-0.0001	-0.0001	-0.0000	681.2410	-0.0000	-0.0000
-0.0000	-0.0001	-0.0001	-0.0000	681.2410	-0.0000
-0.0001	-0.0000	-0.0001	-0.0000	-0.0000	681.2410

[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].