SACADA Database Code: 54

Topology: pbp

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: Im-3m
Pearson: cI48
Coordination Number (CN): 3

Year: 1992

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pbp (SACADA #54)		2.006		0.434	226.1	56.8	9.0	SACADA[1]
6.8^2 P		2.04	Metal					doi: 10.1103/PhysRevLett.68.2325
6.8^2 P								doi: 10.1098/rsta.1993.0045
6.8^2 P								doi: 10.1103/PhysRevB.47.1593
P688		2.28			228			doi: 10.1016/0956-7151(94)90210-0
6.8^2 P								doi: 10.1098/rsta.1996.0088
P688								doi: 10.1016/s0960-8974(97)00003-x
P688								doi: 10.1080/10641229809350239
P688			0.04		273	66.1		doi: 10.1088/1367-2630/5/1/123
P688								doi: 10.1088/1367-2630/5/1/126
BCZ_48								link
pbp								doi: 10.1007/s11224-016-0782-1

Elasticity tensor (kBar)[1]

2927.0857	1927.8240	1927.8240	0.0000	0.0000	-0.0000
1927.8240	2927.0857	1927.8240	0.0000	-0.0000	0.0000
1927.8240	1927.8240	2927.0857	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	618.8552	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	618.8552	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	618.8552

[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].