SACADA Database Code: 53

Topology: pbg

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: Ia-3d
Pearson: cI96
Coordination Number (CN): 3

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pbg (SACADA #53)		2.203		0.400	243.1	94.5	13.7	SACADA[1]
G688								doi: 10.1103/PhysRevB.47.1593
G688		2.28			235			doi: 10.1016/0956-7151(94)90210-0
G688								doi: 10.1016/s0960-8974(97)00003-x
G688								doi: 10.1080/10641229809350239
G688								link
G688								doi: 10.1088/1367-2630/5/1/126
G688			1.5		293	93.3		doi: 10.1088/1367-2630/5/1/123
pbg								doi: 10.1007/s11224-016-0782-1

Elasticity tensor (kBar)[1]

3232.4658	2031.4733	2031.4733	0.0000	0.0000	-0.0000
2031.4733	3232.4658	2031.4733	-0.0000	0.0000	0.0000
2031.4733	2031.4733	3232.4658	0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	1280.5099	-0.0000	-0.0000
0.0000	0.0000	-0.0000	-0.0000	1280.5099	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	1280.5099

[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].