SACADA Database Code: 142

Topology: byl

# of independent nodes (IN): 2
Transitivity: [2663]
Space Group: Imma
Pearson: oI24
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
byl (SACADA #142)		3.420		0.734	424.0	460.6	85.6	SACADA[1]
Imma	0-100	3.373			381	444	87.8	doi: 10.1063/1.4794424
Imma								doi: 10.1016/j.physleta.2014.06.050
Imma								doi: 10.1088/0253-6102/64/2/237
Imma								doi: 10.1007/s10853-015-9266-8

Elasticity tensor (kBar)[1]

10904.2197	826.1227	1129.2201	-0.0000	0.0000	-0.0000
826.1227	10680.4451	553.2930	0.0000	-0.0000	-0.0000
1129.2201	553.2930	11597.0788	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	3585.0955	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	4353.6832	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	5101.2570

[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].