SACADA Database Code: 103

Topology: bbe-3,3-Imma

# of independent nodes (IN): 2
Transitivity: [2331]
Space Group: Imma
Pearson: oI16
Coordination Number (CN): 3

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bbe-3,3-Imma (SACADA #103)		2.607		0.351	222.1	153.7	17.9	SACADA[1]
bco-C16			Semimetal		315			doi: 10.1103/PhysRevLett.116.195501

Elasticity tensor (kBar)[1]

7764.0225	2561.2113	1560.9132	-0.0000	0.0000	-0.0000
2561.2113	9326.1751	597.2241	0.0000	-0.0000	-0.0000
1560.9132	597.2241	1423.8616	-0.0000	0.0000	-0.0000
-0.0000	0.0000	-0.0000	3473.0040	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	847.4576	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	885.7414

[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].