SACADA Database Code: 118

Topology: bba-3,4-P6/mmm

# of independent nodes (IN): 2
Transitivity: [2343]
Space Group: P6/mmm
Pearson: hP12
Coordination Number (CN): 3, 4 (1:1)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bba-3,4-P6/mmm (SACADA #118)		1.682		0.842	193.4	70.1	10.4	SACADA[1]
3D-(6,6)		1.72			195.4	94.1	46.7	doi: 10.1021/nn202053t

Elasticity tensor (kBar)[1]

2247.7609	2105.9442	625.4291	0.0000	-0.0000	0.0000
2105.9442	2247.7609	625.4291	0.0000	0.0000	-0.0000
625.4291	625.4291	6814.4877	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	70.9084	0.0000	-0.0000
-0.0000	0.0000	-0.0000	0.0000	1722.8473	0.0000
0.0000	-0.0000	-0.0000	-0.0000	0.0000	1722.8473

[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].