SACADA Database Code: 126

Topology: sqc3051

# of independent nodes (IN): 2
Transitivity: [2442]
Space Group: P42/mmc
Pearson: tP12
Coordination Number (CN): 3

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sqc3051 (SACADA #126)		1.878		1.069	-	-	-	SACADA[1]
CT-12		1.918			201.4	50.4		doi: 10.1039/c5cp01621e

Elasticity tensor (kBar)[1]

3474.8049	216.6577	1306.2558	-0.0000	-0.0000	0.0000
216.6577	3474.8049	1306.2558	0.0000	0.0000	-0.0000
1306.2558	1306.2558	6069.9630	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	-18.0415	0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	165.6575	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	165.6574

[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].