SACADA Database Code: 473

Topology: 4^4T119

# of independent nodes (IN): 4
Transitivity: [4872]
Space Group: P2/c
Pearson: mP14
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T119 (SACADA #473)		3.251		1.270	353.6	337.5	58.8	SACADA[1]
G181								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8826.3001	1301.0595	774.5686	0.0000	-0.0000	765.6651
1301.0595	6939.1431	1108.2105	0.0000	0.0000	-3.2205
774.5686	1108.2105	9913.4335	-0.0000	0.0000	-621.8811
0.0000	0.0000	-0.0000	3419.9544	77.7526	0.0000
0.0000	0.0000	-0.0000	77.7526	2930.3064	0.0000
765.6651	-3.2205	-621.8811	0.0000	0.0000	3203.8483

[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].