SACADA Database Code: 145

Topology: 4^2T257

# of independent nodes (IN): 2
Transitivity: [2773]
Space Group: P6/mcc
Pearson: hP48
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T257 (SACADA #145)		2.899		0.589	317.5	254.9	36.1	SACADA[1]
3060-carbon		2.855	3.68		307	259	39	doi: 10.1063/1.4955055

Elasticity tensor (kBar)[1]

6084.5203	2161.8162	1008.8302	-0.0000	-0.0000	-0.0000
2161.8162	6084.5203	1008.8302	0.0000	0.0000	0.0000
1008.8302	1008.8302	8081.9139	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	1961.3521	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	2870.7767	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	2870.7767

[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].