SACADA Database Code: 383

Topology: 4^6T33

# of independent nodes (IN): 6
Transitivity: [6(12)71]
Space Group: P21
Pearson: mP12
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
4^6T33 (SACADA #383)		3.268		0.977	369.4	383.1	70.0	SACADA[1]
G64								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9115.5629	1809.4701	1154.0718	0.0000	-0.0000	-345.3024
1809.4701	7980.1752	712.6923	-0.0000	0.0000	588.8658
1154.0718	712.6923	8893.8046	0.0000	-0.0000	-755.9309
-0.0000	-0.0000	0.0000	4105.6086	131.9227	0.0000
-0.0000	0.0000	0.0000	131.9227	3833.4747	-0.0000
-345.3024	588.8658	-755.9309	0.0000	-0.0000	3841.8547

[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].