SACADA Database Code: 194

Topology: 4^3T137

# of independent nodes (IN): 3
Transitivity: [38(11)7]
Space Group: Pmmm
Pearson: oP16
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T137 (SACADA #194)		3.179		1.026	363.8	321.9	52.2	SACADA[1]
(4,0)	255	3.30	5.39		401			doi: 10.1088/1674-1056/24/6/066102

Elasticity tensor (kBar)[1]

9243.2910	583.7021	637.7171	325.1618	9.6811	183.8550
583.7021	10244.1654	939.1205	-394.0760	227.7606	-48.4950
637.7171	939.1205	8982.6130	-18.1280	-167.3053	-136.6040
325.1618	-394.0760	-18.1280	2298.3365	-39.9784	-31.9953
9.6811	227.7606	-167.3053	-39.9784	2702.3898	22.3729
183.8550	-48.4950	-136.6040	-31.9953	22.3729	2893.0952

[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].