SACADA Database Code: 465

Topology: 4^8T41

# of independent nodes (IN): 8
Transitivity: [8(18)(14)5]
Space Group: P-1
Pearson: aP16
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
4^8T41 (SACADA #465)		3.492		0.732	418.1	480.0	90.4	SACADA[1]
G173								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9640.1770	1471.6187	1265.2728	-11.6143	-18.4867	219.3105
1471.6187	9673.5604	935.3554	-136.0511	-129.8058	23.4817
1265.2728	935.3554	11006.2202	176.0022	291.8719	98.5482
-11.6143	-136.0511	176.0022	5004.7136	187.5668	58.7194
-18.4867	-129.8058	291.8719	187.5668	4847.0975	-38.7851
219.3105	23.4817	98.5482	58.7194	-38.7851	5378.1116

[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].