SACADA Database Code: 485

Topology: 4^3T185

# of independent nodes (IN): 3
Transitivity: [3774]
Space Group: C2221
Pearson: oS20
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
4^3T185 (SACADA #485)		3.500		0.990	407.1	475.9	89.9	SACADA[1]
G194								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11173.4130	1128.5121	255.8277	0.0000	0.0000	-0.0000
1128.5121	10424.7146	271.6628	0.0000	0.0000	0.0000
255.8277	271.6628	11741.2593	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	4654.5007	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	4081.1146	0.0000
-0.0000	0.0000	-0.0000	-0.0000	-0.0000	4642.2422

[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].