SACADA Database Code: 182

Topology: 4^3T130

# of independent nodes (IN): 3
Transitivity: [3663]
Space Group: P41212
Pearson: tP20
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
4^3T130 (SACADA #182)		3.435		0.703	430.4	468.9	87.2	SACADA[1]
P41212					413			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

10129.2704	1362.2120	1587.5015	-0.0000	-0.0000	-0.0000
1362.2120	10129.2704	1587.5015	-0.0000	-0.0000	0.0000
1587.5015	1587.5015	9409.8800	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	4511.1188	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	5358.2174	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	5358.2174

[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].