SACADA Database Code: 264

Topology: 4^6T17

# of independent nodes (IN): 6
Transitivity: [6(10)95]
Space Group: Pbam
Pearson: oP24-I
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
4^6T17 (SACADA #264)		3.448		0.638	433.3	486.0	91.1	SACADA[1]
oP24-I	0-20	3.409	4.7		418		91.1	doi: 10.1039/c4cp04569f
Pbam			4.57		416			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

10399.8163	1379.4777	1173.3015	-0.0000	0.0000	-0.0000
1379.4777	11349.1886	331.0372	0.0000	-0.0000	0.0000
1173.3015	331.0372	11478.7863	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	4674.6189	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	4316.4320	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	5298.0653

[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].