SACADA Database Code: 232

Topology: 4^4T106

# of independent nodes (IN): 4
Transitivity: [4(10)62]
Space Group: P43212
Pearson: tP32
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T106 (SACADA #232)		3.593		0.793	388.9	490.6	93.6	SACADA[1]
t32*		3.528	5.23		351			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

10373.2475	490.6460	763.5267	-0.0000	-0.0000	0.0000
490.6460	10373.2475	763.5267	0.0000	-0.0000	-0.0000
763.5267	763.5267	10219.5658	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	4836.5990	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	5025.5772	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	5025.5772

[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].