SACADA Database Code: 237

Topology: 3^5T10

# of independent nodes (IN): 5
Transitivity: [5653]
Space Group: P6/mmm
Pearson: hP30
Coordination Number (CN): 3

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^5T10 (SACADA #237)		1.684		0.762	-	-	-	SACADA[1]
triangular foam		1.67	Metal		145			doi: 10.1039/C0CC05738J

Elasticity tensor (kBar)[1]

3204.2696	1199.1656	951.6714	-0.0000	0.0000	-0.0000
1199.1656	3204.2696	951.6714	0.0000	-0.0000	0.0000
951.6714	951.6714	5628.6770	0.0000	0.0000	0.0000
-0.0000	0.0000	0.0000	1002.5520	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	-199.3885	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	-199.3885

[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].