SACADA Database Code: 265

Topology: 4^6T8

# of independent nodes (IN): 6
Transitivity: [6(12)(11)6]
Space Group: C2/m
Pearson: mS32
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^6T8 (SACADA #265)		3.457		0.686	427.3	485.2	91.2	SACADA[1]
Z-carbon-10			4.24		443		88.1	doi: 10.1021/ja301582d

Elasticity tensor (kBar)[1]

10860.0232	273.2817	1146.2804	-0.0000	0.0000	8.8775
273.2817	11110.5918	1399.1662	-0.0000	0.0000	-1.3527
1146.2804	1399.1662	10882.0933	-0.0000	-0.0000	3.8242
-0.0000	-0.0000	-0.0000	4081.4981	5.2083	0.0000
0.0000	0.0000	0.0000	5.2083	5429.2455	-0.0000
8.8775	-1.3527	3.8242	0.0000	-0.0000	4877.2172

[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].