SACADA Database Code: 284

Topology: 4^7T10

# of independent nodes (IN): 7
Transitivity: [7(14)(14)8]
Space Group: C2/m
Pearson: mS40
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T10 (SACADA #284)		3.473		0.665	429.6	492.0	92.6	SACADA[1]
20C	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11219.4387	270.6593	1385.8022	-0.0000	-0.0000	-5.4078
270.6593	10940.4708	1189.2435	0.0000	0.0000	4.2931
1385.8022	1189.2435	10840.1222	0.0000	0.0000	-3.8603
-0.0000	0.0000	-0.0000	4175.8403	1.1876	-0.0000
-0.0000	0.0000	0.0000	1.1876	5033.6075	-0.0000
-5.4078	4.2931	-3.8603	-0.0000	-0.0000	5466.1450

[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].