SACADA Database Code: 312

Topology: 4^{10}T8

# of independent nodes (IN): 10
Transitivity: [(10)(15)(14)9]
Space Group: Pmn21
Pearson: oP20
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^{10}T8 (SACADA #312)		3.478		0.648	416.0	481.2	90.8	SACADA[1]
20A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11158.6966	477.5196	961.4937	-0.0000	0.0000	-0.0000
477.5196	10607.8254	803.6879	0.0000	-0.0000	-0.0000
961.4937	803.6879	11225.3198	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	4223.3429	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	4492.9977	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	5186.1847

[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].