SACADA Database Code: 323

Topology: 4^{11}T9

# of independent nodes (IN): 11
Transitivity: [(11)(24)(20)8]
Space Group: P-1
Pearson: aP22
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^{11}T9 (SACADA #323)		3.507		0.693	421.5	489.7	92.5	SACADA[1]
22C	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

9825.6122	1267.4285	1430.7962	-171.9813	3.2632	-33.0599
1267.4285	11183.2075	729.2052	-59.2763	-250.8492	140.5233
1430.7962	729.2052	10094.9292	-11.2766	249.1477	-139.2485
-171.9813	-59.2763	-11.2766	5458.7496	-16.8828	-6.9182
3.2632	-250.8492	249.1477	-16.8828	4759.5554	-115.4202
-33.0599	140.5233	-139.2485	-6.9182	-115.4202	5148.1291

[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].