SACADA Database Code: 21

Topology: bsn

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: I41/amd
Pearson: tI4
Coordination Number (CN): 6

Year: 1983

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bsn (SACADA #21)		3.545		0.000	447.9	528.1	100.0	SACADA[1]
beta-tin								doi: 10.1103/PhysRevLett.50.2006
beta-tin								link

Elasticity tensor (kBar)[1]

11786.4407	273.2345	1381.6322	0.0000	0.0000	-0.0000
273.2345	11786.4407	1381.6322	-0.0000	-0.0000	0.0000
1381.6322	1381.6322	10662.3413	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	4640.9411	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	5754.6867	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	5754.6866

[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].