SACADA Database Code: 350

Topology: 4^{22}T1

# of independent nodes (IN): 22
Transitivity: [(22)(33)(31)(20)]
Space Group: Pm
Pearson: mP22
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^{22}T1 (SACADA #350)		3.465		0.635	418.0	483.9	91.3	SACADA[1]
22A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10737.3949	938.1571	675.9362	-0.0000	-0.0000	-81.3547
938.1571	11216.6864	444.3614	0.0000	0.0000	77.8503
675.9362	444.3614	11558.0938	0.0000	0.0000	-3.1411
-0.0000	0.0000	0.0000	4998.5528	77.6173	-0.0000
-0.0000	0.0000	0.0000	77.6173	4615.8482	-0.0000
-81.3547	77.8503	-3.1411	-0.0000	-0.0000	4193.4871

[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].