SACADA Database Code: 334

Topology: 4^{14}T1

# of independent nodes (IN): 14
Transitivity: [(14)(21)(19)(12)]
Space Group: Pm
Pearson: mP14
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^{14}T1 (SACADA #334)		3.420		0.674	410.1	469.1	88.3	SACADA[1]
14B	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10302.5281	908.9425	757.6571	-0.0000	-0.0000	93.7751
908.9425	11107.2815	378.9503	-0.0000	-0.0000	-115.9269
757.6571	378.9503	11420.8633	0.0000	0.0000	-61.5858
-0.0000	-0.0000	0.0000	4894.6901	-143.2175	-0.0000
-0.0000	-0.0000	0.0000	-143.2175	4480.0580	0.0000
93.7751	-115.9269	-61.5858	-0.0000	0.0000	3954.1475

[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].