SACADA Database Code: 343

Topology: 4^{18}T2

# of independent nodes (IN): 18
Transitivity: [(18)(27)(25)(16)]
Space Group: Cm
Pearson: mS36
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^{18}T2 (SACADA #343)		3.445		0.658	414.6	479.5	90.5	SACADA[1]
18B	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

11723.9978	299.8771	625.5419	-0.0000	-0.0000	142.3496
299.8771	11239.3401	949.0928	0.0000	0.0000	119.8587
625.5419	949.0928	10611.2797	0.0000	0.0000	-203.1360
-0.0000	0.0000	0.0000	4437.9128	196.5769	0.0000
-0.0000	0.0000	0.0000	196.5769	5033.1732	0.0000
142.3496	119.8587	-203.1360	0.0000	0.0000	4083.0980

[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].