SACADA Database Code: 338

Topology: 4^{16}T4

# of independent nodes (IN): 16
Transitivity: [(16)(26)(25)(15)]
Space Group: P2/m
Pearson: mP32
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{16}T4 (SACADA #338)		3.499		0.613	420.7	491.1	92.8	SACADA[1]
10(I)								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

10830.2382	278.9465	1260.9049	-0.0000	0.0000	-0.4233
278.9465	11248.3756	1208.3277	0.0000	0.0000	-1.4622
1260.9049	1208.3277	10293.9373	-0.0000	-0.0000	-5.4976
-0.0000	0.0000	-0.0000	4324.8452	-0.0378	0.0000
0.0000	0.0000	-0.0000	-0.0378	5358.7540	0.0000
-0.4233	-1.4622	-5.4976	0.0000	0.0000	5101.5840

[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].