SACADA Database Code: 336

Topology: 4^{16}T3

# of independent nodes (IN): 16
Transitivity: [(16)(24)(22)(14)]
Space Group: Pm
Pearson: mP16
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^{16}T3 (SACADA #336)		3.459		0.668	413.6	475.5	89.6	SACADA[1]
16D	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10420.0662	426.1362	949.3325	-0.0000	-0.0000	89.4552
426.1362	11111.9111	984.5747	0.0000	0.0000	27.5282
949.3325	984.5747	11004.9830	0.0000	-0.0000	-367.6909
-0.0000	0.0000	0.0000	4105.1096	-87.3419	0.0000
-0.0000	0.0000	-0.0000	-87.3419	5181.5053	0.0000
89.4552	27.5282	-367.6909	0.0000	0.0000	4523.8429

[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].