SACADA Database Code: 330

Topology: 4^{13}T3

# of independent nodes (IN): 13
Transitivity: [(13)(17)(16)(13)]
Space Group: Cmcm
Pearson: oS72
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^{13}T3 (SACADA #330)		3.504		0.608	422.0	493.5	93.3	SACADA[1]
8(I)								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11261.6948	1213.9283	281.6473	-0.0000	0.0000	-0.0000
1213.9283	10316.8380	1260.1224	-0.0000	-0.0000	-0.0000
281.6473	1260.1224	10890.1570	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	5380.3769	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	5144.0119	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	-0.0000	4349.6736

[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].