SACADA Database Code: 310

Topology: 4^{10}T9

# of independent nodes (IN): 10
Transitivity: [(10)(13)(13)10]
Space Group: Cmcm
Pearson: oS56
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^{10}T9 (SACADA #310)		3.493		0.620	419.0	487.8	92.1	SACADA[1]
6(I)			4.042(D)					doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11217.0833	1192.9604	282.8603	0.0000	0.0000	0.0000
1192.9604	10276.4829	1255.6814	0.0000	-0.0000	0.0000
282.8603	1255.6814	10755.3576	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	5326.9966	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	5034.8578	-0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	4289.6938

[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].