SACADA Database Code: 288

Topology: $3,4^7T1$

# of independent nodes (IN): 8
Transitivity: [8998]
Space Group: Cmmm
Pearson: oS32
Coordination Number (CN): 3, 4 (1:7)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^7T1$ (SACADA #288)		3.443		0.663	427.8	400.3	68.6	SACADA[1]
16C	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10787.7241	1647.4027	1444.1565	-0.0000	-0.0000	-0.0000
1647.4027	9219.3929	337.8136	-0.0000	-0.0000	-0.0000
1444.1565	337.8136	11880.6707	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	2315.9096	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	3660.5168	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	5563.2456

[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].