SACADA Database Code: 248

Topology: $3^2,4^3$T64

# of independent nodes (IN): 5
Transitivity: [5(10)71]
Space Group: P-1
Pearson: aP10
Coordination Number (CN): 3, 4 (1:1)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^3$T64 (SACADA #248)		3.022		0.500	330.2	296.2	48.7	SACADA[1]
C_{10}-C		3.07	1.25					doi: 10.1016/j.carbon.2016.08.015

Elasticity tensor (kBar)[1]

6647.7599	1280.2630	1296.1176	978.5802	-342.0220	-658.9376
1280.2630	7808.6047	1224.5571	1781.3050	1237.5347	459.3725
1296.1176	1224.5571	8173.1378	158.0595	844.4485	-1072.0232
978.5802	1781.3050	158.0595	3125.9413	-25.5056	-112.2763
-342.0220	1237.5347	844.4485	-25.5056	3153.2129	756.8178
-658.9376	459.3725	-1072.0232	-112.2763	756.8178	2596.9078

[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].