SACADA Database Code: 380

Topology: 4^2T10

# of independent nodes (IN): 2
Transitivity: [2551]
Space Group: C2/c
Pearson: mS16
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T10 (SACADA #380)		3.155		0.959	359.5	334.5	57.1	SACADA[1]
G60								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

7604.8231	1378.6713	1165.0348	5.8464	-116.1898	1.5745
1378.6713	8638.0986	1073.2655	7.4800	-702.2659	-3.6728
1165.0348	1073.2655	8924.1383	3.7932	861.0392	0.9028
5.8464	7.4800	3.7932	2461.5931	-2.4416	860.6843
-116.1898	-702.2659	861.0392	-2.4416	3698.6924	0.4932
1.5745	-3.6728	0.9028	860.6843	0.4932	4078.0909

[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].