SACADA Database Code: 246

Topology: 4^5T27

# of independent nodes (IN): 5
Transitivity: [5984]
Space Group: C2/m
Pearson: mS20
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^5T27 (SACADA #246)		3.389		0.730	413.7	456.6	85.3	SACADA[1]
10A	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

9537.2677	394.2039	1170.6645	0.0000	0.0000	453.5369
394.2039	11207.8303	1005.4088	-0.0000	-0.0000	-293.5233
1170.6645	1005.4088	11529.6977	-0.0000	0.0000	9.7039
0.0000	-0.0000	-0.0000	3584.9671	-218.1697	0.0000
0.0000	-0.0000	0.0000	-218.1697	5301.5324	0.0000
453.5369	-293.5233	9.7039	0.0000	0.0000	4302.8554

[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].