SACADA Database Code: 222

Topology: 4^4T32

# of independent nodes (IN): 4
Transitivity: [4764]
Space Group: Imma
Pearson: oI24
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T32 (SACADA #222)		3.418		0.705	419.2	472.8	88.7	SACADA[1]
Z-CACB		3.365	4.196		405.41		82.01	doi: 10.1039/c2cp40531h
Z-CACB								doi: 10.3103/s1063457612060123
12E								doi: 10.1103/PhysRevB.88.014102
Z-CACB								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11265.3945	260.3784	1276.2198	-0.0000	-0.0000	-0.0000
260.3784	10259.7755	1144.6610	0.0000	0.0000	0.0000
1276.2198	1144.6610	10918.6695	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	3886.8100	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	4670.5452	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	5320.9218

[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].