SACADA Database Code: 52

Topology: gis

# of independent nodes (IN): 1
Transitivity: [1231]
Space Group: I41/amd
Pearson: tI16
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
gis (SACADA #52)		2.666		0.786	290.0	186.1	21.2	SACADA[1]
LA8								doi: 10.1134/s1063776111060173
LA8								link

Elasticity tensor (kBar)[1]

3891.1499	1903.8634	2335.2716	-0.0000	-0.0000	-0.0000
1903.8634	3891.1499	2335.2716	0.0000	0.0000	-0.0000
2335.2716	2335.2716	5880.5130	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	2084.4378	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	2852.5595	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	2852.5596

[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].