SACADA Database Code: 87

Topology: mer

# of independent nodes (IN): 1
Transitivity: [1463]
Space Group: I4/mmm
Pearson: tI32
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
mer (SACADA #87)		2.648		0.846	276.3	190.9	22.2	SACADA[1]
CA5								doi: 10.1134/s1063776111060173
CA5								link

Elasticity tensor (kBar)[1]

6864.0687	1283.3350	1515.4866	0.0000	-0.0000	-0.0000
1283.3350	6864.0687	1515.4866	-0.0000	-0.0000	0.0000
1515.4866	1515.4866	3549.6096	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	1019.0463	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	2493.0140	-0.0000
-0.0000	0.0000	-0.0000	0.0000	-0.0000	2493.0140

[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].