SACADA Database Code: 56

Topology: uni

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: P6122
Pearson: hP6
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
uni (SACADA #56)		3.474		0.663	414.2	486.4	92.0	SACADA[1]
uni								doi: 10.1524/zkri.2013.1620

Elasticity tensor (kBar)[1]

10282.4010	1339.9622	260.0707	-0.0000	-0.0000	-0.0000
1339.9622	10282.4010	260.0707	-0.0000	0.0000	0.0000
260.0707	260.0707	13074.4531	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	4471.2194	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	4714.7168	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	4714.7162

[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].