SACADA Database Code: 57

Topology: unc

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: P4122
Pearson: tP4
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
unc (SACADA #57)		3.426		1.087	392.5	372.1	64.5	SACADA[1]
G		3.387						doi: 10.1103/PhysRevB.70.045101
unc								doi: 10.1524/zkri.2013.1620

Elasticity tensor (kBar)[1]

7017.6705	2456.5298	798.6775	0.0000	-0.0000	-0.0000
2456.5298	7017.6705	798.6775	-0.0000	0.0000	-0.0000
798.6775	798.6775	14007.3675	0.0000	-0.0000	-0.0000
0.0000	-0.0000	0.0000	2673.1798	-0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	4557.3953	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	4557.3953

[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].