SACADA Database Code: 29

Topology: unj

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: P6122
Pearson: hP6
Coordination Number (CN): 4

Year: 2002

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
unj (SACADA #29)		3.249		0.695	402.3	420.0	76.9	SACADA[1]
								doi: 10.1021/jp014115g
CFS			4.12		390			doi: 10.1103/PhysRevB.81.014106
unj								doi: 10.1039/c004039h
CFS			4.02		413			doi: 10.1103/PhysRevB.83.035206
unj								doi: 10.1524/zkri.2013.1620
6A								doi: 10.1103/PhysRevB.88.014102
P6522					389			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

9294.2390	1868.4387	1349.7964	-0.0000	-0.0000	-0.0000
1868.4387	9294.2390	1349.7964	-0.0000	0.0000	0.0000
1349.7964	1349.7964	8552.9154	-0.0000	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	3712.9001	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	4989.3105	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	4989.3112

[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].