SACADA Database Code: 114

Topology: sqc326

# of independent nodes (IN): 2
Transitivity: [2333]
Space Group: Immm
Pearson: oI12
Coordination Number (CN): 3

Year: 1999

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sqc326 (SACADA #114)		2.365		1.047	-	-	-	SACADA[1]
New polymorph		2.4	Metal		234			doi: 10.1016/s0009-2614(99)00943-4
6(3)4-25		2.41						doi: 10.1016/S0009-2614(01)00126-9

Elasticity tensor (kBar)[1]

2909.3628	2906.2914	703.9581	-0.0000	-0.0000	-0.0000
2906.2914	5115.9278	1317.5336	-0.0000	0.0000	0.0000
703.9581	1317.5336	7270.5549	0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	2003.1740	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	1118.3942	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	-199.6960

[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].