SACADA Database Code: 236

Topology: 3^5T2

# of independent nodes (IN): 5
Transitivity: [5632]
Space Group: Imm2
Pearson: oI12
Coordination Number (CN): 3

Year: 2001

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^5T2 (SACADA #236)		2.214		1.357	228.7	64.9	10.1	SACADA[1]
6(3)3-27		2.24						doi: 10.1016/S0009-2614(01)00126-9

Elasticity tensor (kBar)[1]

3350.6425	460.9273	1032.1091	-0.0000	0.0000	0.0000
460.9273	4594.4962	2013.2122	-0.0000	-0.0000	-0.0000
1032.1091	2013.2122	7466.7085	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	70.4004	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	570.7523	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	565.7686

[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].