SACADA Database Code: 90

Topology: twt

# of independent nodes (IN): 1
Transitivity: -
Space Group: P6222
Pearson: hP6
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
twt (SACADA #90)		3.395		1.384	-	-	-	SACADA[1]
6(3)1-06		3.41						doi: 10.1016/S0009-2614(01)00126-9

Elasticity tensor (kBar)[1]

10085.0979	1497.6720	1980.2165	0.0000	-0.0000	-0.0000
1497.6720	10085.0979	1980.2165	0.0000	0.0000	-0.0000
1980.2165	1980.2165	5314.2930	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	4293.7130	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	-2487.5063	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	-2487.5067

[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].