SACADA Database Code: 216

Topology: 3^4T13

# of independent nodes (IN): 3
Transitivity: [4674]
Space Group: Ia-3d
Pearson: cI384
Coordination Number (CN): 3

Year: 1992

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^4T13 (SACADA #216)		1.239		0.762	130.7	64.0	8.4	SACADA[1]
G8								doi: 10.1016/0008-6223(92)90066-6
G8								doi: 10.1098/rsta.1993.0045
G8								doi: 10.1016/0009-2614(93)85009-d
G8								link
G8		1.23			134			doi: 10.1016/0956-7151(94)90210-0
G8								link
G8								doi: 10.1016/s0960-8974(97)00003-x
G8			0.2		159	69.0		doi: 10.1088/1367-2630/5/1/123
G8								doi: 10.1088/1367-2630/5/1/126

Elasticity tensor (kBar)[1]

2017.8120	950.5400	950.5400	0.0000	-0.0000	-0.0000
950.5400	2017.8120	950.5400	-0.0000	0.0000	0.0000
950.5400	950.5400	2017.8120	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	722.3570	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	722.3570	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	722.3570

[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].