SACADA Database Code: 157

Topology: 3^3T5

# of independent nodes (IN): 3
Transitivity: [3432]
Space Group: Cmmm
Pearson: oS12
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
3^3T5 (SACADA #157)		2.451		1.203	144.9	88.2	10.2	SACADA[1]
6(3)3-26		2.48	0.99					doi: 10.1016/S0009-2614(01)00126-9

Elasticity tensor (kBar)[1]

10206.3941	557.2014	1066.6531	0.0000	0.0000	-0.0000
557.2014	5578.6099	-19.1518	0.0000	0.0000	0.0000
1066.6531	-19.1518	7089.5799	-0.0000	-0.0000	-0.0000
0.0000	0.0000	-0.0000	1085.6097	-0.0000	0.0000
0.0000	0.0000	-0.0000	-0.0000	169.8197	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	468.2430

[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].