SACADA Database Code: 208

Topology: 3^4T14

# of independent nodes (IN): 4
Transitivity: [4542]
Space Group: P42/mmc
Pearson: tP16
Coordination Number (CN): 3

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^4T14 (SACADA #208)		2.809		1.455	-	-	-	SACADA[1]
GT-16		2.960			347.6	135.1		doi: 10.1039/c5cp01621e

Elasticity tensor (kBar)[1]

6895.6121	471.3445	236.7435	0.0000	0.0000	-0.0000
471.3445	6895.6121	236.7435	-0.0000	0.0000	-0.0000
236.7435	236.7435	4691.3524	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	-285.4985	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	-1044.5775	-0.0000
-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-1044.5775

[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].