SACADA Database Code: 461

Topology: 4^{16}T18

# of independent nodes (IN): 16
Transitivity: [(16)(24)(21)(13)]
Space Group: Im
Pearson: mS32
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^{16}T18 (SACADA #461)		3.377		0.799	386.4	430.2	80.5	SACADA[1]
G169								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9296.9134	960.0210	1330.3569	0.0000	0.0000	236.9250
960.0210	10654.8159	472.6638	0.0000	-0.0000	135.3406
1330.3569	472.6638	9318.5059	0.0000	-0.0000	287.3066
0.0000	0.0000	0.0000	4748.3504	505.5593	0.0000
0.0000	-0.0000	-0.0000	505.5593	3960.7461	-0.0000
236.9250	135.3406	287.3066	0.0000	-0.0000	4058.9682

[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].