SACADA Database Code: 460

Topology: 4^5T59

# of independent nodes (IN): 5
Transitivity: [5(10)(10)5]
Space Group: P2/c
Pearson: mP16
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
4^5T59 (SACADA #460)		3.381		0.926	390.2	427.0	79.5	SACADA[1]
G167								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8512.1590	1282.5347	1592.9582	-0.0000	-0.0000	4.2228
1282.5347	9948.4987	892.7446	-0.0000	-0.0000	174.2238
1592.9582	892.7446	9139.6588	0.0000	0.0000	156.8968
-0.0000	-0.0000	0.0000	5022.5731	67.2485	0.0000
-0.0000	-0.0000	0.0000	67.2485	4149.2062	0.0000
4.2228	174.2238	156.8968	0.0000	0.0000	4365.7254

[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].