SACADA Database Code: 414

Topology: 4^5T56

# of independent nodes (IN): 5
Transitivity: [5(12)(10)5]
Space Group: P-1
Pearson: aP10
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
4^5T56 (SACADA #414)		3.487		0.838	416.0	473.3	89.0	SACADA[1]
G112								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11976.2362	404.1043	772.6135	102.6435	156.1183	-215.9824
404.1043	10124.1015	1206.9417	350.6411	-844.3060	26.9220
772.6135	1206.9417	10636.9612	6.6903	503.8765	-517.1861
102.6435	350.6411	6.6903	4203.0180	-362.2158	203.7561
156.1183	-844.3060	503.8765	-362.2158	4474.6609	301.5630
-215.9824	26.9220	-517.1861	203.7561	301.5630	5119.9843

[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].