SACADA Database Code: 513

Topology: 4^3T189

# of independent nodes (IN): 3
Transitivity: [3983]
Space Group: P21/m
Pearson: mP12
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
4^3T189 (SACADA #513)		3.235		0.870	375.4	382.2	69.3	SACADA[1]
G228								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10733.3731	619.3618	959.5068	0.0000	0.0000	374.8067
619.3618	9802.8250	670.8158	-0.0000	0.0000	-394.1522
959.5068	670.8158	8845.9939	0.0000	0.0000	457.2172
-0.0000	-0.0000	0.0000	3749.1540	428.8299	-0.0000
0.0000	-0.0000	0.0000	428.8299	3418.6244	-0.0000
374.8067	-394.1522	457.2172	-0.0000	-0.0000	3130.7941

[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].