SACADA Database Code: 481

Topology: 4^3T183

# of independent nodes (IN): 3
Transitivity: [3774]
Space Group: C2/c
Pearson: mS20
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
4^3T183 (SACADA #481)		3.173		1.199	344.6	323.5	55.6	SACADA[1]
G189								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8330.2460	1352.9785	865.6658	0.0000	0.0000	-128.8013
1352.9785	7533.1663	1457.8430	0.0000	0.0000	349.4893
865.6658	1457.8430	7806.1806	0.0000	-0.0000	-933.3379
0.0000	-0.0000	0.0000	2875.2936	-44.3628	0.0000
0.0000	-0.0000	-0.0000	-44.3628	4061.3598	-0.0000
-128.8013	349.4893	-933.3379	0.0000	-0.0000	2752.1506

[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].