SACADA Database Code: 410

Topology: 4^4T114

# of independent nodes (IN): 4
Transitivity: [4973]
Space Group: C2/m
Pearson: mS24
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
4^4T114 (SACADA #410)		3.278		0.969	371.6	409.8	76.5	SACADA[1]
G104								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8653.1012	822.7551	888.9705	0.0000	-0.0000	327.3409
822.7551	10295.8678	689.1146	-0.0000	0.0000	-326.0723
888.9705	689.1146	9757.3779	0.0000	-0.0000	-190.5443
0.0000	-0.0000	0.0000	3867.1223	-393.4079	-0.0000
-0.0000	0.0000	-0.0000	-393.4079	3612.7596	0.0000
327.3409	-326.0723	-190.5443	-0.0000	0.0000	4330.3277

[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].