SACADA Database Code: 412

Topology: 4^4T116

# of independent nodes (IN): 4
Transitivity: [4773]
Space Group: C2/m
Pearson: mS16
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
4^4T116 (SACADA #412)		3.313		0.868	367.2	381.8	69.8	SACADA[1]
G107								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10421.6886	472.9248	443.4196	0.0000	0.0000	825.3845
472.9248	10462.5664	773.2247	0.0000	0.0000	-9.3833
443.4196	773.2247	8872.0028	0.0000	0.0000	224.1829
0.0000	0.0000	0.0000	4121.7761	359.0655	-0.0000
0.0000	0.0000	0.0000	359.0655	3779.1120	-0.0000
825.3845	-9.3833	224.1829	-0.0000	-0.0000	2418.3559

[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].