SACADA Database Code: 519

Topology: 4^3T191

# of independent nodes (IN): 3
Transitivity: [39(11)5]
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
4^3T191 (SACADA #519)		3.355		0.987	371.9	376.3	68.0	SACADA[1]
G238								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10174.9868	1143.1240	700.3074	0.0000	-0.0000	170.9648
1143.1240	7828.7731	721.2885	-0.0000	-0.0000	337.1911
700.3074	721.2885	10570.9130	0.0000	-0.0000	203.9670
-0.0000	-0.0000	0.0000	2878.1083	391.7370	0.0000
-0.0000	-0.0000	-0.0000	391.7370	3165.0317	0.0000
170.9648	337.1911	203.9670	0.0000	-0.0000	4503.5933

[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].