SACADA Database Code: 379

Topology: 4^4T86

# of independent nodes (IN): 4
Transitivity: [4863]
Space Group: I2/a
Pearson: mS28
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
4^4T86 (SACADA #379)		3.424		0.777	411.0	452.9	84.5	SACADA[1]
G59								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9354.1142	1515.3199	1302.7499	0.0000	0.0000	156.5761
1515.3199	9218.4557	1380.7883	-0.0000	-0.0000	-79.2742
1302.7499	1380.7883	10041.6662	-0.0000	0.0000	528.7013
0.0000	-0.0000	-0.0000	4883.1478	441.9266	-0.0000
0.0000	-0.0000	0.0000	441.9266	4990.1399	-0.0000
156.5761	-79.2742	528.7013	-0.0000	-0.0000	4733.2178

[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].