SACADA Database Code: 515

Topology: 4^4T125

# of independent nodes (IN): 4
Transitivity: [4951]
Space Group: P2/m1
Pearson: mP16
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
4^4T125 (SACADA #515)		3.431		0.785	407.5	456.8	85.6	SACADA[1]
G230								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10439.2400	1331.3578	759.8437	0.0000	0.0000	-91.0916
1331.3578	9121.6804	1469.6468	0.0000	-0.0000	4.3780
759.8437	1469.6468	10005.7810	-0.0000	-0.0000	374.4201
0.0000	0.0000	-0.0000	5291.4407	33.2237	-0.0000
0.0000	0.0000	-0.0000	33.2237	4503.5261	0.0000
-91.0916	4.3780	374.4201	-0.0000	-0.0000	4480.3806

[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].