SACADA Database Code: 365

Topology: 4^5T49

# of independent nodes (IN): 5
Transitivity: [5884]
Space Group: P21/m
Pearson: mP10
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
4^5T49 (SACADA #365)		3.380		0.693	403.3	444.8	83.0	SACADA[1]
G21								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9629.5107	869.8553	1199.6780	-0.0000	-0.0000	65.7330
869.8553	10805.0772	515.6133	-0.0000	0.0000	-211.5108
1199.6780	515.6133	10706.0250	-0.0000	0.0000	-139.6808
-0.0000	-0.0000	-0.0000	4654.6745	-490.9716	0.0000
-0.0000	0.0000	0.0000	-490.9716	4482.5342	0.0000
65.7330	-211.5108	-139.6808	0.0000	0.0000	3707.2326

[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].