SACADA Database Code: 245

Topology: 4^5T13

# of independent nodes (IN): 5
Transitivity: [5974]
Space Group: P21/m
Pearson: mP10
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^5T13 (SACADA #245)		3.408		0.773	417.5	463.9	86.8	SACADA[1]
P21/m	25.0						85.4	doi: 10.1063/1.4794424

Elasticity tensor (kBar)[1]

10963.5522	315.8396	1099.9583	0.0000	-0.0000	423.7610
315.8396	11115.8519	1118.1782	0.0000	-0.0000	-65.2422
1099.9583	1118.1782	10432.9042	-0.0000	0.0000	374.5196
0.0000	0.0000	-0.0000	3960.2546	226.3221	0.0000
-0.0000	-0.0000	0.0000	226.3221	5303.7215	0.0000
423.7610	-65.2422	374.5196	0.0000	0.0000	4119.4200

[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].