SACADA Database Code: 280

Topology: 4^7T9

# of independent nodes (IN): 7
Transitivity: [7(12)(10)6]
Space Group: P21/m
Pearson: mP14
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
4^7T9 (SACADA #280)		3.414		0.688	425.0	482.5	90.7	SACADA[1]
14D	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10769.8932	981.3170	613.2800	0.0000	-0.0000	-36.8283
981.3170	11555.6083	289.2522	0.0000	-0.0000	-110.7727
613.2800	289.2522	12170.0526	-0.0000	0.0000	139.0922
0.0000	0.0000	-0.0000	5083.0989	-178.4720	-0.0000
-0.0000	-0.0000	0.0000	-178.4720	4435.7327	0.0000
-36.8283	-110.7727	139.0922	-0.0000	0.0000	3947.2111

[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].