SACADA Database Code: 272

Topology: 4^7T14

# of independent nodes (IN): 7
Transitivity: [7(10)97]
Space Group: Cmcm
Pearson: oS40
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T14 (SACADA #272)		3.470		0.641	430.8	490.5	92.2	SACADA[1]
4(I)			4.09(D)					doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11489.8705	1270.6677	299.3506	0.0000	-0.0000	0.0000
1270.6677	10558.5549	1367.2529	0.0000	0.0000	0.0000
299.3506	1367.2529	10856.7713	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	5405.0266	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	5017.9456	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	4232.6757

[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].