SACADA Database Code: 678

Topology: 4^4T4-CA

# of independent nodes (IN): 4
Transitivity: [4763]
Space Group: Pnnm
Pearson: oP16
Coordination Number (CN): 4

Year: 2023

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T4-CA (SACADA #678)		3.396		0.156	412.5	453.0	84.4	SACADA[1]
4^4T4-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10757.9260	1363.6119	1039.7360	0.0000	0.0000	0.0000
1363.6119	9463.1403	568.0229	-0.0000	-0.0000	-0.0000
1039.7360	568.0229	11049.1099	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	4551.0678	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	3926.8654	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	4833.6457

[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].