SACADA Database Code: 672

Topology: 4^4T3-CA

# of independent nodes (IN): 4
Transitivity: [4(10)84]
Space Group: P21/n
Pearson: mP16
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
4^4T3-CA (SACADA #672)		3.496		0.428	419.7	476.0	89.4	SACADA[1]
4^4T3-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

12433.2581	675.9836	455.9581	-0.0000	0.0000	-6.7143
675.9836	10748.8006	868.8497	-0.0000	0.0000	-210.1653
455.9581	868.8497	10647.7218	-0.0000	-0.0000	65.9190
-0.0000	-0.0000	-0.0000	5067.5754	-32.7087	-0.0000
0.0000	0.0000	-0.0000	-32.7087	3928.1045	-0.0000
-6.7143	-210.1653	65.9190	-0.0000	-0.0000	4393.9447

[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].