SACADA Database Code: 667

Topology: 4^4T34-CA

# of independent nodes (IN): 4
Transitivity: [4(13)(10)5]
Space Group: P2/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
4^4T34-CA (SACADA #667)		3.485		0.898	371.8	284.4	37.3	SACADA[1]
4^4T34-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

12285.4376	66.6586	394.3313	0.0000	0.0000	-91.3962
66.6586	8241.0085	625.0943	0.0000	-0.0000	-824.3237
394.3313	625.0943	11234.4788	-0.0000	-0.0000	-836.2320
0.0000	0.0000	-0.0000	1664.8396	-2507.5460	-0.0000
0.0000	-0.0000	-0.0000	-2507.5460	1033.4776	-0.0000
-91.3962	-824.3237	-836.2320	-0.0000	-0.0000	4202.9399

[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].