SACADA Database Code: 687

Topology: 4^4T5-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
4^4T5-CA (SACADA #687)		3.378		0.705	370.9	376.5	68.1	SACADA[1]
4^4T5-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10204.4235	487.6301	130.8123	0.0000	-0.0000	913.8694
487.6301	8666.6451	1337.1206	-0.0000	0.0000	-233.4643
130.8123	1337.1206	10677.3074	0.0000	-0.0000	328.5627
-0.0000	-0.0000	0.0000	2496.6791	623.7101	-0.0000
-0.0000	0.0000	-0.0000	623.7101	3484.6398	0.0000
913.8694	-233.4643	328.5627	0.0000	0.0000	4206.6177

[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].