SACADA Database Code: 669

Topology: 4^4T36-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(12)5]
Space Group: P21/m
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
4^4T36-CA (SACADA #669)		3.293		0.322	389.1	391.4	70.5	SACADA[1]
4^4T36-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10945.2442	499.9926	793.0191	-0.0000	-0.0000	353.3799
499.9926	10809.0638	572.0299	-0.0000	-0.0000	-280.4102
793.0191	572.0299	9587.1811	0.0000	-0.0000	361.6794
0.0000	-0.0000	0.0000	3869.6988	369.7574	0.0000
-0.0000	0.0000	-0.0000	369.7574	3557.1279	-0.0000
353.3799	-280.4102	361.6794	0.0000	-0.0000	2778.2537

[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].