SACADA Database Code: 659

Topology: 4^4T24-CA

# of independent nodes (IN): 4
Transitivity: [4(12)(12)5]
Space Group: Pccn
Pearson: oP32
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
4^4T24-CA (SACADA #659)		3.515		0.295	432.5	501.2	94.6	SACADA[1]
4^4T24-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11447.8275	684.9897	1204.3116	0.0000	-0.0000	-0.0000
684.9897	12046.8075	204.3228	-0.0000	0.0000	0.0000
1204.3116	204.3228	11251.0534	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	5078.8112	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	4220.4308	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	5013.2176

[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].