SACADA Database Code: 657

Topology: 4^4T22-CA

# of independent nodes (IN): 4
Transitivity: [4(12)(12)5]
Space Group: Pbcm
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
4^4T22-CA (SACADA #657)		3.291		0.324	387.6	388.6	69.9	SACADA[1]
4^4T22-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9521.7791	777.5462	596.4717	-0.0000	0.0000	-0.0000
777.5462	10932.4621	521.6946	-0.0000	0.0000	0.0000
596.4717	521.6946	10694.8336	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	2705.1272	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	3918.8882	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	3537.8219

[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].