SACADA Database Code: 674

Topology: 4^4T42-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(11)6]
Space Group: Pmna
Pearson: oP28
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
4^4T42-CA (SACADA #674)		3.490		0.390	419.4	479.8	90.3	SACADA[1]
4^4T42-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10859.3858	470.4677	797.8939	0.0000	-0.0000	0.0000
470.4677	11818.5290	115.8281	0.0000	0.0000	0.0000
797.8939	115.8281	12324.9410	0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	3981.2405	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	4479.8073	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	4557.5926

[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].