SACADA Database Code: 646

Topology: 4^4T12-CA

# of independent nodes (IN): 4
Transitivity: [4842]
Space Group: R-3c
Pearson: hR96
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
4^4T12-CA (SACADA #646)		3.300		0.278	395.2	420.8	77.7	SACADA[1]
4^4T12-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10414.3001	789.0998	907.7694	1.4774	-241.8986	0.7462
789.0998	10422.3483	906.9197	0.9558	242.6779	1.1609
907.7694	906.9197	9549.9505	7.5849	-0.6516	-3.4298
1.4774	0.9558	7.5849	4815.9091	0.2853	-242.3680
-241.8986	242.6779	-0.6516	0.2853	3590.4331	0.6512
0.7462	1.1609	-3.4298	-242.3680	0.6512	3592.3456

[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].