SACADA Database Code: 647

Topology: 4^4T13-CA

# of independent nodes (IN): 4
Transitivity: [4842]
Space Group: R-3
Pearson: hR48
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
4^4T13-CA (SACADA #647)		3.330		0.269	406.4	426.9	78.4	SACADA[1]
4^4T13-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10630.1530	875.6513	1078.1310	2.6763	320.1778	-151.8647
875.6513	10619.4574	1077.5738	0.7193	-319.7913	154.1874
1078.1310	1077.5738	9309.9869	15.9807	0.1432	-3.9917
2.6763	0.7193	15.9807	4877.6218	158.1380	322.1730
320.1778	-319.7913	0.1432	158.1380	3742.3005	4.9405
-151.8647	154.1874	-3.9917	322.1730	4.9405	3746.9276

[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].