SACADA Database Code: 663

Topology: 4^4T29-CA

# of independent nodes (IN): 4
Transitivity: [4961]
Space Group: Pmn21
Pearson: oP16
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
4^4T29-CA (SACADA #663)		3.095		0.425	369.4	317.9	49.8	SACADA[1]
4^4T29-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9487.0847	1143.2192	1137.9000	-0.0000	-0.0000	-0.0000
1143.2192	8132.0679	1446.6582	0.0000	-0.0000	-0.0000
1137.9000	1446.6582	8209.3836	0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	3198.9377	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	2062.0377	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	3690.3531

[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].