SACADA Database Code: 702

Topology: 4^4T9-CA

# of independent nodes (IN): 4
Transitivity: [4972]
Space Group: P21/n
Pearson: mP16
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
4^4T9-CA (SACADA #702)		3.336		0.847	348.6	188.2	23.3	SACADA[1]
4^4T9-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9001.3783	-24.7078	828.3815	0.0000	0.0000	648.2917
-24.7078	9377.7044	1474.6108	0.0000	0.0000	4.9419
828.3815	1474.6108	8481.5565	-0.0000	0.0000	-150.4672
0.0000	0.0000	0.0000	3825.1277	108.8403	0.0000
0.0000	0.0000	0.0000	108.8403	3769.3241	0.0000
648.2917	4.9419	-150.4672	-0.0000	0.0000	3037.7323

[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].