SACADA Database Code: 693

Topology: 4^4T66-CA

# of independent nodes (IN): 4
Transitivity: [4961]
Space Group: P3221
Pearson: hP24
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
4^4T66-CA (SACADA #693)		3.482		0.481	412.8	457.7	85.5	SACADA[1]
4^4T66-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11379.7877	1045.8074	867.2223	1.8444	-238.4639	-0.0177
1045.8074	11374.2945	878.2223	-1.3984	237.8885	1.0959
867.2223	878.2223	9045.1764	9.4708	2.2786	1.3884
1.8444	-1.3984	9.4708	5176.8768	4.4595	-241.0764
-238.4639	237.8885	2.2786	4.4595	4108.3688	4.1346
-0.0177	1.0959	1.3884	-241.0764	4.1346	4107.3517

[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].