SACADA Database Code: 684

Topology: 4^4T56-CA

# of independent nodes (IN): 4
Transitivity: [4(11)84]
Space Group: C2/c
Pearson: mS32
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
4^4T56-CA (SACADA #684)		3.393		0.478	398.9	436.2	81.2	SACADA[1]
4^4T56-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10864.6195	450.8892	649.4803	-0.0000	0.0000	474.8835
450.8892	10312.2926	1478.0524	0.0000	0.0000	181.2649
649.4803	1478.0524	9572.5940	-0.0000	-0.0000	715.0138
-0.0000	0.0000	-0.0000	3833.3753	792.6330	-0.0000
0.0000	0.0000	-0.0000	792.6330	4288.0890	0.0000
474.8835	181.2649	715.0138	0.0000	0.0000	4408.3960

[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].