SACADA Database Code: 683

Topology: 4^4T55-CA

# of independent nodes (IN): 4
Transitivity: [4(11)84]
Space Group: I2/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
4^4T55-CA (SACADA #683)		3.351		0.526	390.4	407.4	74.6	SACADA[1]
4^4T55-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9133.7304	1462.0860	823.1156	-0.0000	0.0000	758.8309
1462.0860	10200.7970	584.7965	-0.0000	0.0000	222.3162
823.1156	584.7965	10086.0288	0.0000	0.0000	74.8123
-0.0000	-0.0000	0.0000	3958.1836	846.3708	0.0000
0.0000	0.0000	0.0000	846.3708	3828.6358	-0.0000
758.8309	222.3162	74.8123	0.0000	-0.0000	3808.3664

[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].