SACADA Database Code: 686

Topology: 4^4T58-CA

# of independent nodes (IN): 4
Transitivity: [4(11)85]
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
4^4T58-CA (SACADA #686)		3.353		0.350	382.0	443.1	83.6	SACADA[1]
4^4T58-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10293.3714	723.6656	951.9006	-0.0000	-0.0000	685.8829
723.6656	9030.8063	1275.6013	-0.0000	0.0000	-128.9817
951.9006	1275.6013	9174.5553	-0.0000	0.0000	175.4668
-0.0000	-0.0000	-0.0000	4253.9464	-184.2476	-0.0000
-0.0000	0.0000	0.0000	-184.2476	4975.0129	0.0000
685.8829	-128.9817	175.4668	0.0000	0.0000	4486.1934

[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].