SACADA Database Code: 644

Topology: 4^4T10-CA

# of independent nodes (IN): 4
Transitivity: [4(10)94]
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
4^4T10-CA (SACADA #644)		3.475		0.552	405.5	448.8	83.8	SACADA[1]
4^4T10-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10207.8243	662.1263	1597.5526	0.0000	0.0000	623.5665
662.1263	11729.3551	389.8470	-0.0000	0.0000	-167.3190
1597.5526	389.8470	9325.1284	-0.0000	-0.0000	-660.3488
0.0000	-0.0000	-0.0000	4604.6489	228.8493	-0.0000
0.0000	0.0000	-0.0000	228.8493	4088.5492	0.0000
623.5665	-167.3190	-660.3488	-0.0000	0.0000	4344.6928

[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].