SACADA Database Code: 675

Topology: 4^4T43-CA

# of independent nodes (IN): 4
Transitivity: [4(10)(10)6]
Space Group: I212121
Pearson: oI28
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
4^4T43-CA (SACADA #675)		3.490		0.388	419.2	477.9	89.9	SACADA[1]
4^4T43-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11753.6962	539.9535	69.9639	-0.0000	0.0000	0.0000
539.9535	10733.6354	866.1995	-0.0000	-0.0000	-0.0000
69.9639	866.1995	12321.6651	0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	4000.7350	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	4581.8368	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	4426.7753

[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].