SACADA Database Code: 697

Topology: 4^4T70-CA

# of independent nodes (IN): 4
Transitivity: [4(10)94]
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
4^4T70-CA (SACADA #697)		3.468		0.564	402.5	452.5	84.8	SACADA[1]
4^4T70-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10419.5604	460.4937	1440.9328	0.0000	-0.0000	522.7195
460.4937	12137.6253	467.7446	-0.0000	0.0000	25.3871
1440.9328	467.7446	9054.5532	0.0000	0.0000	-639.3056
-0.0000	-0.0000	0.0000	4379.7756	90.8627	-0.0000
-0.0000	0.0000	0.0000	90.8627	4320.4619	0.0000
522.7195	25.3871	-639.3056	-0.0000	0.0000	4330.6628

[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].