SACADA Database Code: 676

Topology: 4^4T45-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(11)6]
Space Group: C2/m
Pearson: mS28
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
4^4T45-CA (SACADA #676)		3.481		0.375	415.5	481.5	90.9	SACADA[1]
4^4T45-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

12572.2367	756.4400	212.2825	-0.0000	-0.0000	410.2413
756.4400	10810.4799	289.9254	0.0000	-0.0000	-6.4654
212.2825	289.9254	11570.9203	0.0000	-0.0000	-88.7619
-0.0000	0.0000	-0.0000	4631.9926	60.2404	-0.0000
-0.0000	0.0000	0.0000	60.2404	3950.7802	-0.0000
410.2413	-6.4654	-88.7619	0.0000	-0.0000	4501.8184

[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].