SACADA Database Code: 650

Topology: 4^4T16-CA

# of independent nodes (IN): 4
Transitivity: [4994]
Space Group: P21/n
Pearson: mP16
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
4^4T16-CA (SACADA #650)		3.527		0.309	437.0	503.5	94.9	SACADA[1]
4^4T16-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11125.7549	784.3753	638.7550	0.0000	-0.0000	175.8697
784.3753	12650.2594	789.6022	0.0000	0.0000	-124.7698
638.7550	789.6022	11211.0998	-0.0000	0.0000	-460.6444
0.0000	0.0000	-0.0000	5215.0266	-391.3817	-0.0000
-0.0000	0.0000	0.0000	-391.3817	5144.2923	0.0000
175.8697	-124.7698	-460.6444	-0.0000	0.0000	4059.1468

[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].