SACADA Database Code: 668

Topology: 4^4T35-CA

# of independent nodes (IN): 4
Transitivity: [4(12)(14)9]
Space Group: P2/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
4^4T35-CA (SACADA #668)		3.471		0.900	394.8	439.7	82.3	SACADA[1]
4^4T35-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

12731.6377	185.4194	335.1291	0.0000	-0.0000	201.8775
185.4194	9742.2552	978.7974	0.0000	-0.0000	-88.3615
335.1291	978.7974	10183.9255	-0.0000	-0.0000	515.6536
0.0000	-0.0000	-0.0000	3691.1207	88.9753	0.0000
0.0000	0.0000	-0.0000	88.9753	3904.6859	0.0000
201.8775	-88.3615	515.6536	0.0000	0.0000	4302.1913

[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].