SACADA Database Code: 638

Topology: 4^3T196-CA

# of independent nodes (IN): 3
Transitivity: [3653]
Space Group: Cmca
Pearson: oS32
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
4^3T196-CA (SACADA #638)		3.441		0.482	396.0	438.4	81.9	SACADA[1]
4^3T196-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9187.3989	537.7835	1752.2846	-0.0000	0.0000	-0.0000
537.7835	11335.6120	432.4267	0.0000	-0.0000	-0.0000
1752.2846	432.4267	9692.3589	0.0000	-0.0000	-0.0000
-0.0000	0.0000	0.0000	4093.9339	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	4575.1548	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	4229.1014

[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].