SACADA Database Code: 641

Topology: 4^3T204-CA

# of independent nodes (IN): 3
Transitivity: [3684]
Space Group: Pcca
Pearson: oP16
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
4^3T204-CA (SACADA #641)		3.391		1.199	377.6	284.8	36.5	SACADA[1]
4^3T204-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

14070.1091	672.7045	656.0309	0.0000	-0.0000	0.0000
672.7045	7064.4913	2275.2956	0.0000	-0.0000	0.0000
656.0309	2275.2956	6582.9393	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	3913.6148	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	1242.1198	-0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	2935.2085

[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].