SACADA Database Code: 682

Topology: 4^4T53-CA

# of independent nodes (IN): 4
Transitivity: [4(12)(12)6]
Space Group: P2221
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
4^4T53-CA (SACADA #682)		3.493		0.364	421.5	482.7	90.9	SACADA[1]
4^4T53-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11803.9417	436.1489	190.4894	0.0000	0.0000	0.0000
436.1489	10920.4058	828.2711	-0.0000	0.0000	0.0000
190.4894	828.2711	12341.7548	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	3970.6252	-0.0000	0.0000
0.0000	0.0000	0.0000	-0.0000	4629.1498	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	4562.4086

[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].