SACADA Database Code: 655

Topology: 4^4T20-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(11)5]
Space Group: Pnma
Pearson: oP32
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
4^4T20-CA (SACADA #655)		3.341		0.241	407.0	426.5	78.3	SACADA[1]
4^4T20-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9440.0805	892.6674	1994.3714	-0.0000	-0.0000	-0.0000
892.6674	10889.5981	199.4105	0.0000	-0.0000	0.0000
1994.3714	199.4105	10127.9967	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	3565.6782	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	4163.9499	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	4679.4345

[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].