SACADA Database Code: 635

Topology: 4^3T193-CA

# of independent nodes (IN): 3
Transitivity: [3663]
Space Group: P2221
Pearson: oP8
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
4^3T193-CA (SACADA #635)		3.431		0.620	383.0	396.4	72.4	SACADA[1]
4^3T193-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

8664.6889	1791.9016	541.3853	0.0000	0.0000	0.0000
1791.9016	7994.9596	800.9706	-0.0000	0.0000	0.0000
541.3853	800.9706	11724.9515	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	3210.2782	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	4624.8700	-0.0000
0.0000	0.0000	0.0000	-0.0000	-0.0000	3933.1592

[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].