SACADA Database Code: 639

Topology: 4^3T197-CA

# of independent nodes (IN): 3
Transitivity: [3883]
Space Group: Pnma
Pearson: oP24
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
4^3T197-CA (SACADA #639)		3.269		0.344	391.6	387.7	69.2	SACADA[1]
4^3T197-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9163.4997	873.0227	1645.3276	-0.0000	-0.0000	0.0000
873.0227	10272.1826	504.2098	-0.0000	0.0000	-0.0000
1645.3276	504.2098	9766.5556	-0.0000	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	3562.0620	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	3865.7664	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	0.0000	3378.9996

[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].