SACADA Database Code: 633

Topology: 4^3T191-CA

# of independent nodes (IN): 3
Transitivity: [3553]
Space Group: Ibca
Pearson: oI32
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
4^3T191-CA (SACADA #633)		3.483		0.477	417.2	454.9	84.6	SACADA[1]
4^3T191-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

8727.4870	1710.6785	550.5251	2.7112	0.4984	-2.4207
1710.6785	10184.1134	807.9318	1.2452	0.1981	-0.5942
550.5251	807.9318	12752.3015	1.3422	-0.3354	0.0480
2.7112	1.2452	1.3422	4187.0705	-1.0871	-0.8258
0.4984	0.1981	-0.3354	-1.0871	5127.9910	1.8777
-2.4207	-0.5942	0.0480	-0.8258	1.8777	4165.6506

[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].