SACADA Database Code: 666

Topology: 4^4T32-CA

# of independent nodes (IN): 4
Transitivity: [4972]
Space Group: P21/c
Pearson: mP16
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
4^4T32-CA (SACADA #666)		3.560		1.129	393.6	436.4	81.5	SACADA[1]
4^4T32-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

7450.1705	121.6487	1840.8504	-0.0000	0.0000	-480.6038
121.6487	14558.0003	518.9946	-0.0000	-0.0000	-186.4475
1840.8504	518.9946	9242.0214	0.0000	-0.0000	-402.8247
0.0000	-0.0000	0.0000	4008.1922	-477.3961	-0.0000
0.0000	-0.0000	-0.0000	-477.3961	4898.0404	0.0000
-480.6038	-186.4475	-402.8247	-0.0000	0.0000	3964.8124

[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].