SACADA Database Code: 658

Topology: 4^4T23-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(11)5]
Space Group: Pccn
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
4^4T23-CA (SACADA #658)		3.529		0.856	408.5	463.0	87.0	SACADA[1]
4^4T23-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

13461.4666	228.8648	390.5342	-0.0000	0.0000	-0.0000
228.8648	10159.0422	1083.5413	0.0000	0.0000	0.0000
390.5342	1083.5413	9929.3260	-0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	4465.4698	0.0000	-0.0000
0.0000	-0.0000	0.0000	0.0000	3962.6160	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	4380.2322

[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].