SACADA Database Code: 554

Topology: 4^3T50-CA

# of independent nodes (IN): 3
Transitivity: [39(10)4]
Space Group: Pnnm
Pearson: oP24
Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T50-CA (SACADA #554)		3.333		0.482	396.5	411.0	75.1	SACADA[1]
4^3T50-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

11481.3224	211.1135	537.5317	-0.0000	0.0000	-0.0000
211.1135	9149.1515	2343.9779	-0.0000	-0.0000	-0.0000
537.5317	2343.9779	8873.8734	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	4222.2389	-0.0000	-0.0000
0.0000	0.0000	-0.0000	-0.0000	4115.2616	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	3694.4871

[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].