SACADA Database Code: 551

Topology: 4^3T37-CA

# of independent nodes (IN): 3
Transitivity: [3(10)93]
Space Group: Pbcm
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
4^3T37-CA (SACADA #551)		3.419		0.165	424.1	460.1	85.5	SACADA[1]
4^3T37-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10679.4003	1142.8047	1011.5880	0.0000	-0.0000	0.0000
1142.8047	11585.7871	564.9325	-0.0000	-0.0000	-0.0000
1011.5880	564.9325	10501.8193	-0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	5093.9783	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	4384.2286	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	3701.1020

[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].