SACADA Database Code: 588

Topology: 4^3T164-CA

# of independent nodes (IN): 3
Transitivity: [3992]
Space Group: C2/m
Pearson: mS24
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
4^3T164-CA (SACADA #588)		3.046		0.428	359.0	293.8	42.8	SACADA[1]
4^3T164-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8040.2885	2864.3501	772.0163	-0.0000	0.0000	-27.5218
2864.3501	4980.4914	1847.4855	0.0000	0.0000	283.1280
772.0163	1847.4855	8681.8206	0.0000	0.0000	-159.4596
-0.0000	0.0000	0.0000	3451.7281	139.8300	0.0000
0.0000	0.0000	0.0000	139.8300	2870.5261	-0.0000
-27.5218	283.1280	-159.4596	0.0000	0.0000	3885.1816

[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].