SACADA Database Code: 582

Topology: 4^3T158-CA

# of independent nodes (IN): 3
Transitivity: [3894]
Space Group: Pnma
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
4^3T158-CA (SACADA #582)		3.062		0.588	304.9	287.4	49.6	SACADA[1]
4^3T158-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9158.8858	1025.0765	1421.1845	-0.0000	-0.0000	-0.0000
1025.0765	3948.1271	1321.3029	-0.0000	-0.0000	0.0000
1421.1845	1321.3029	8880.5184	0.0000	0.0000	0.0000
-0.0000	0.0000	0.0000	2414.4285	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	2704.7125	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	3825.2904

[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].