SACADA Database Code: 583

Topology: 4^3T159-CA

# of independent nodes (IN): 3
Transitivity: [39(10)6]
Space Group: I2/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
4^3T159-CA (SACADA #583)		3.321		0.206	404.0	432.5	80.0	SACADA[1]
4^3T159-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9279.6810	309.0659	1354.5212	-0.0000	-0.0000	-432.6380
309.0659	11589.9241	476.4405	-0.0000	-0.0000	-13.6335
1354.5212	476.4405	11358.3619	-0.0000	0.0000	1084.7371
-0.0000	-0.0000	0.0000	3539.2981	121.4474	0.0000
-0.0000	0.0000	0.0000	121.4474	4242.0074	-0.0000
-432.6380	-13.6335	1084.7371	0.0000	-0.0000	4072.3298

[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].