SACADA Database Code: 569

Topology: 4^3T83-CA

# of independent nodes (IN): 3
Transitivity: [3862]
Space Group: P6522
Pearson: hP36
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
4^3T83-CA (SACADA #569)		3.421		0.194	422.5	485.5	91.5	SACADA[1]
4^3T83-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10895.3385	868.8724	859.2211	-0.0000	0.0000	0.0000
868.8724	10895.3385	859.2211	-0.0000	-0.0000	-0.0000
859.2211	859.2211	11067.4105	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	5013.2331	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	4597.5816	0.0000
0.0000	-0.0000	-0.0000	-0.0000	0.0000	4597.5816

[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].