SACADA Database Code: 559

Topology: 4^3T56-CA

# of independent nodes (IN): 3
Transitivity: [39(10)5]
Space Group: Pcca
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
4^3T56-CA (SACADA #559)		3.553		1.059	374.4	397.0	73.2	SACADA[1]
4^3T56-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10547.1730	862.9322	803.5437	-0.0000	-0.0000	0.0000
862.9322	8330.8688	277.7019	-0.0000	-0.0000	-0.0000
803.5437	277.7019	11227.2459	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	3588.6494	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	2720.7189	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	4678.9819

[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].