SACADA Database Code: 610

Topology: 4^3T187-CA

# of independent nodes (IN): 3
Transitivity: [3883]
Space Group: Cmmm
Pearson: oS32
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
4^3T187-CA (SACADA #610)		3.226		0.439	362.6	350.6	61.6	SACADA[1]
4^3T187-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10140.8351	803.5425	1462.8925	0.0000	-0.0000	0.0000
803.5425	6911.4438	776.5742	0.0000	0.0000	0.0000
1462.8925	776.5742	10183.1719	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	2956.5906	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	2722.1575	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	4154.7589

[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].