SACADA Database Code: 572

Topology: 4^3T147-CA

# of independent nodes (IN): 3
Transitivity: [3862]
Space Group: Pnna
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
4^3T147-CA (SACADA #572)		3.223		0.321	388.5	391.6	70.6	SACADA[1]
4^3T147-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8958.1848	795.2739	1792.8761	-0.0000	0.0000	-0.0000
795.2739	9091.2246	1196.7435	-0.0000	0.0000	-0.0000
1792.8761	1196.7435	9403.6535	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	3810.9838	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	4126.0919	0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	3787.4202

[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].