SACADA Database Code: 560

Topology: 4^3T57-CA

# of independent nodes (IN): 3
Transitivity: [3752]
Space Group: P21/c
Pearson: mP12
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
4^3T57-CA (SACADA #560)		3.244		0.577	346.8	358.3	65.4	SACADA[1]
4^3T57-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8537.7770	615.8150	837.6338	-0.0000	-0.0000	-123.4814
615.8150	8013.7576	1416.9961	-0.0000	-0.0000	23.2401
837.6338	1416.9961	8985.1648	-0.0000	0.0000	-774.1197
-0.0000	-0.0000	-0.0000	2813.0914	-79.6172	-0.0000
-0.0000	-0.0000	0.0000	-79.6172	4494.0449	-0.0000
-123.4814	23.2401	-774.1197	-0.0000	-0.0000	3295.0413

[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].