SACADA Database Code: 567

Topology: 4^3T64-CA

# of independent nodes (IN): 3
Transitivity: [3795]
Space Group: P21212
Pearson: oP12
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
4^3T64-CA (SACADA #567)		3.320		0.711	384.3	376.2	66.7	SACADA[1]
4^3T64-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9649.9700	833.3781	1486.3521	0.0000	-0.0000	-0.0000
833.3781	7438.4575	2580.0815	0.0000	0.0000	0.0000
1486.3521	2580.0815	7762.9657	-0.0000	0.0000	-0.0000
-0.0000	0.0000	-0.0000	3981.0637	0.0000	-0.0000
-0.0000	0.0000	0.0000	0.0000	4232.0330	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	4364.7423

[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].