SACADA Database Code: 568

Topology: 4^3T75-CA

# of independent nodes (IN): 3
Transitivity: [3773]
Space Group: Imma
Pearson: oI24
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
4^3T75-CA (SACADA #568)		3.391		0.199	415.0	439.2	80.9	SACADA[1]
4^3T75-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10186.5496	494.2718	2209.0968	-0.0000	-0.0000	-0.0000
494.2718	11217.1910	888.6193	-0.0000	-0.0000	0.0000
2209.0968	888.6193	8796.5250	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	4165.3871	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	4867.5450	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	4259.7807

[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].