SACADA Database Code: 556

Topology: 4^3T52-CA

# of independent nodes (IN): 3
Transitivity: [39(10)6]
Space Group: I2/m
Pearson: mS24
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
4^3T52-CA (SACADA #556)		3.446		0.451	410.5	446.8	83.1	SACADA[1]
4^3T52-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

12046.4845	460.8522	298.0470	0.0000	-0.0000	-278.3689
460.8522	10109.2477	991.9658	-0.0000	-0.0000	-121.4820
298.0470	991.9658	11329.2832	0.0000	0.0000	225.0532
0.0000	-0.0000	0.0000	3955.0806	-152.7923	0.0000
-0.0000	-0.0000	0.0000	-152.7923	3599.3440	-0.0000
-278.3689	-121.4820	225.0532	-0.0000	-0.0000	4506.1121

[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].