SACADA Database Code: 563

Topology: 4^3T60-CA

# of independent nodes (IN): 3
Transitivity: [3543]
Space Group: P63/mcm
Pearson: hP24
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
4^3T60-CA (SACADA #563)		3.363		0.288	395.0	406.9	74.1	SACADA[1]
4^3T60-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10764.0074	1294.9179	763.9575	0.0045	-0.0000	-0.0000
1294.9179	10763.9985	763.9572	0.0045	0.0000	0.0000
763.9575	763.9572	8642.2897	0.0003	0.0000	0.0000
0.0045	0.0045	0.0003	4734.5425	0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	3380.8070	0.0014
-0.0000	0.0000	0.0000	-0.0000	0.0014	3380.8086

[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].