SACADA Database Code: 565

Topology: 4^3T62-CA

# of independent nodes (IN): 3
Transitivity: [3785]
Space Group: P21/n
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
4^3T62-CA (SACADA #565)		3.097		0.829	335.9	326.8	57.7	SACADA[1]
4^3T62-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

7170.2718	728.1508	830.7377	0.0000	-0.0000	-1587.2085
728.1508	10739.0106	1053.7222	-0.0000	-0.0000	1.8043
830.7377	1053.7222	7561.0768	-0.0000	0.0000	-646.7671
0.0000	-0.0000	-0.0000	3378.4658	-765.2067	-0.0000
-0.0000	-0.0000	0.0000	-765.2067	4249.9408	0.0000
-1587.2085	1.8043	-646.7671	-0.0000	-0.0000	1878.1472

[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].