SACADA Database Code: 561

Topology: 4^3T58-CA

# of independent nodes (IN): 3
Transitivity: [3774]
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
4^3T58-CA (SACADA #561)		3.272		0.988	357.9	341.8	59.5	SACADA[1]
4^3T58-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9183.5489	2156.4577	898.8409	-0.0000	0.0000	219.6637
2156.4577	6577.7315	844.6137	0.0000	-0.0000	-661.8928
898.8409	844.6137	8956.0320	0.0000	-0.0000	458.5390
-0.0000	0.0000	0.0000	4068.3517	-438.2960	0.0000
0.0000	-0.0000	-0.0000	-438.2960	2723.4331	0.0000
219.6637	-661.8928	458.5390	0.0000	0.0000	3691.9355

[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].