SACADA Database Code: 587

Topology: 4^3T163-CA

# of independent nodes (IN): 3
Transitivity: [3972]
Space Group: C2/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
4^3T163-CA (SACADA #587)		3.274		0.312	392.8	381.5	67.3	SACADA[1]
4^3T163-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9473.8107	1733.6058	1152.4789	0.0000	0.0000	115.8988
1733.6058	7723.2971	1011.8620	-0.0000	-0.0000	60.7170
1152.4789	1011.8620	10554.6517	0.0000	0.0000	94.9685
0.0000	-0.0000	0.0000	3228.1369	160.9748	0.0000
0.0000	-0.0000	0.0000	160.9748	3506.9628	-0.0000
115.8988	60.7170	94.9685	0.0000	-0.0000	4634.6938

[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].