SACADA Database Code: 585

Topology: 4^3T161-CA

# of independent nodes (IN): 3
Transitivity: [39(10)5]
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
4^3T161-CA (SACADA #585)		3.175		0.377	371.9	339.5	56.9	SACADA[1]
4^3T161-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8978.1003	2125.4520	1051.3065	-0.0000	0.0000	203.4727
2125.4520	5912.1801	1550.4261	0.0000	0.0000	210.7755
1051.3065	1550.4261	9577.8024	-0.0000	-0.0000	219.8328
-0.0000	0.0000	-0.0000	3301.2084	505.9718	0.0000
0.0000	0.0000	-0.0000	505.9718	3152.7693	-0.0000
203.4727	210.7755	219.8328	0.0000	-0.0000	4381.5872

[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].