SACADA Database Code: 584

Topology: 4^3T160-CA

# of independent nodes (IN): 3
Transitivity: [3994]
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
4^3T160-CA (SACADA #584)		3.166		0.402	367.2	336.7	56.7	SACADA[1]
4^3T160-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9098.1045	2018.3197	1162.2356	0.0000	0.0000	-91.5160
2018.3197	5848.1198	1386.9059	0.0000	0.0000	182.5763
1162.2356	1386.9059	9536.2739	0.0000	-0.0000	-278.7714
-0.0000	-0.0000	0.0000	3352.9321	-79.2680	-0.0000
0.0000	0.0000	-0.0000	-79.2680	3023.6902	0.0000
-91.5160	182.5763	-278.7714	-0.0000	0.0000	4205.9123

[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].