SACADA Database Code: 581

Topology: 4^3T157-CA

# of independent nodes (IN): 3
Transitivity: [3863]
Space Group: Cmcm
Pearson: oS32
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
4^3T157-CA (SACADA #581)		3.341		0.256	402.7	414.1	75.4	SACADA[1]
4^3T157-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10371.0624	1109.3959	1075.3672	-0.0000	0.0000	0.0000
1109.3959	10905.5871	1132.4502	0.0000	-0.0000	-0.0000
1075.3672	1132.4502	8525.6603	-0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	4746.0743	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	3999.2896	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	3334.0544

[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].