SACADA Database Code: 576

Topology: 4^3T151-CA

# of independent nodes (IN): 3
Transitivity: [3861]
Space Group: Pnma
Pearson: oP24
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
4^3T151-CA (SACADA #576)		3.273		0.314	391.8	384.8	68.3	SACADA[1]
4^3T151-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10579.9735	1213.9640	1030.5177	0.0000	-0.0000	0.0000
1213.9640	7705.0215	1469.0324	0.0000	0.0000	-0.0000
1030.5177	1469.0324	9771.7617	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	3589.0689	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	3240.6190	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	4513.3338

[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].