SACADA Database Code: 577

Topology: 4^3T152-CA

# of independent nodes (IN): 3
Transitivity: [3(10)82]
Space Group: Pmna
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
4^3T152-CA (SACADA #577)		3.269		0.309	392.7	381.8	67.4	SACADA[1]
4^3T152-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

7429.3997	1597.3776	1399.4330	0.0000	-0.0000	0.0000
1597.3776	9418.6857	1061.2937	-0.0000	0.0000	-0.0000
1399.4330	1061.2937	10635.8241	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	3023.3427	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	4502.5335	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	4043.1210

[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].