SACADA Database Code: 532

Topology: 4^2T22-CA

# of independent nodes (IN): 2
Transitivity: [2542]
Space Group: P6122
Pearson: hP18
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
4^2T22-CA (SACADA #532)		3.469		0.566	395.6	445.1	83.5	SACADA[1]
4^2T22-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10227.8473	1059.4622	1244.2059	-0.0029	-0.0000	0.0000
1059.4622	10227.8392	1244.2054	-0.0029	-0.0000	0.0000
1244.2059	1244.2054	8210.4904	-0.0004	-0.0000	0.0000
-0.0029	-0.0029	-0.0004	4584.1905	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	4698.3439	-0.0013
0.0000	0.0000	0.0000	0.0000	-0.0013	4698.3457

[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].