SACADA Database Code: 548

Topology: 4^3T22-CA

# of independent nodes (IN): 3
Transitivity: [3763]
Space Group: P63/m
Pearson: hP28
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
4^3T22-CA (SACADA #548)		3.385		0.201	418.2	440.6	81.0	SACADA[1]
4^3T22-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

10925.2857	1072.8569	923.4265	0.7752	-0.0614	-0.2153
1072.8569	10917.9211	924.0371	0.7483	-0.3244	0.1526
923.4265	924.0371	9998.0486	1.1317	-1.1593	0.1751
0.7752	0.7483	1.1317	4925.6148	4.6836	0.1093
-0.0614	-0.3244	-1.1593	4.6836	3812.3164	2.0535
-0.2153	0.1526	0.1751	0.1093	2.0535	3815.3866

[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].