SACADA Database Code: 544

Topology: 4^2T45-CA

# of independent nodes (IN): 2
Transitivity: [2774]
Space Group: P-4m2
Pearson: tP16
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
4^2T45-CA (SACADA #544)		2.760		0.984	251.6	148.8	17.4	SACADA[1]
4^2T45-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

4079.2634	977.6508	1452.2447	-0.0000	-0.0000	-0.0000
977.6508	4079.2634	1452.2447	-0.0000	0.0000	-0.0000
1452.2447	1452.2447	7990.5123	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	1254.0642	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	1219.4719	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	1219.4718

[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].