SACADA Database Code: 546

Topology: 4^2T168

# of independent nodes (IN): 2
Transitivity: [2684]
Space Group: C2/m
Pearson: mS16
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
4^2T168 (SACADA #546)		3.229		0.346	382.5	364.5	63.4	SACADA[1]
4^2T168								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9277.8671	1860.9638	1087.1734	-0.0000	-0.0000	271.8509
1860.9638	6890.8966	1271.6077	-0.0000	-0.0000	-57.5173
1087.1734	1271.6077	10103.4685	0.0000	0.0000	465.3965
0.0000	-0.0000	0.0000	3310.6937	512.6407	0.0000
0.0000	-0.0000	0.0000	512.6407	3322.6381	0.0000
271.8509	-57.5173	465.3965	0.0000	0.0000	4525.1924

[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].