SACADA Database Code: 533

Topology: 4^2T31-CA

# of independent nodes (IN): 2
Transitivity: [2793]
Space Group: I41/amd
Pearson: tI64
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
4^2T31-CA (SACADA #533)		3.211		0.805	345.5	307.5	50.2	SACADA[1]
4^2T31-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

8793.9820	1419.8185	352.9936	0.0000	0.0000	0.0000
1419.8185	8793.9820	352.9936	0.0000	-0.0000	-0.0000
352.9936	352.9936	9265.6759	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	2038.9370	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	2830.4026	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	2830.4026

[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].