SACADA Database Code: 552

Topology: 4^3T48-CA

# of independent nodes (IN): 3
Transitivity: [3774]
Space Group: Immm
Pearson: oI24
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
4^3T48-CA (SACADA #552)		2.988		0.832	250.8	205.5	30.0	SACADA[1]
4^3T48-CA								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

2655.1020	717.5629	572.2473	-0.0000	0.0000	0.0000
717.5629	8215.1793	2358.6300	-0.0000	-0.0000	-0.0000
572.2473	2358.6300	8486.0789	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	1412.2953	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	2962.1917	0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	1558.7176

[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].