SACADA Database Code: 652

Topology: 4^4T18-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(11)5]
Space Group: Pnma
Pearson: oP32
Coordination Number (CN): 4

Year: 2023

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T18-CA (SACADA #652)		3.349		0.236	406.0	432.4	79.8	SACADA[1]
4^4T18-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10838.3964	240.7333	1837.4399	-0.0000	0.0000	-0.0000
240.7333	11081.5448	689.7790	-0.0000	-0.0000	-0.0000
1837.4399	689.7790	9138.1955	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	4231.9528	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	3526.7093	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	4668.7339

[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].