SACADA Database Code: 670

Topology: 4^4T37-CA

# of independent nodes (IN): 4
Transitivity: [4884]
Space Group: Cmca
Pearson: oS48
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
4^4T37-CA (SACADA #670)		3.507		0.904	388.2	384.8	68.7	SACADA[1]
4^4T37-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

8532.4627	1143.4514	456.8381	-0.0000	0.0000	0.0000
1143.4514	10868.2132	157.5567	0.0000	0.0000	0.0000
456.8381	157.5567	12255.5938	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	3027.2258	0.0000	0.0000
0.0000	0.0000	0.0000	-0.0000	3855.5794	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	2981.8300

[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].