SACADA Database Code: 673

Topology: 4^4T40-CA

# of independent nodes (IN): 4
Transitivity: [4(10)72]
Space Group: C2/m
Pearson: mS24
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
4^4T40-CA (SACADA #673)		3.442		0.356	412.9	471.6	88.8	SACADA[1]
4^4T40-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11193.7335	1109.0783	872.1552	0.0000	0.0000	103.1344
1109.0783	10542.8046	439.4783	0.0000	-0.0000	391.8984
872.1552	439.4783	10627.5457	-0.0000	-0.0000	-43.5556
-0.0000	0.0000	0.0000	5363.7159	279.3476	0.0000
0.0000	0.0000	-0.0000	279.3476	3764.0168	0.0000
103.1344	391.8984	-43.5556	0.0000	-0.0000	4656.0477

[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].