SACADA Database Code: 688

Topology: 4^4T60-CA

# of independent nodes (IN): 4
Transitivity: [4951]
Space Group: P21/n
Pearson: mP16
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
4^4T60-CA (SACADA #688)		3.431		0.294	419.5	464.5	86.8	SACADA[1]
4^4T60-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11667.1464	1068.7301	567.2962	0.0000	-0.0000	224.3585
1068.7301	9250.8825	1287.4025	0.0000	-0.0000	-374.1871
567.2962	1287.4025	11086.5973	0.0000	-0.0000	320.9003
0.0000	0.0000	0.0000	4586.5883	-76.9311	0.0000
0.0000	0.0000	-0.0000	-76.9311	4298.3486	-0.0000
224.3585	-374.1871	320.9003	0.0000	-0.0000	4747.0638

[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].