SACADA Database Code: 691

Topology: 4^4T64-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(10)4]
Space Group: P2/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
4^4T64-CA (SACADA #691)		3.331		0.483	383.8	396.0	72.2	SACADA[1]
4^4T64-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11116.0033	741.4372	526.2515	0.0000	-0.0000	408.6703
741.4372	9040.7022	814.4650	0.0000	-0.0000	-493.5643
526.2515	814.4650	10306.8832	0.0000	-0.0000	413.9487
0.0000	0.0000	0.0000	3198.8668	113.0097	0.0000
-0.0000	0.0000	-0.0000	113.0097	3137.2674	0.0000
408.6703	-493.5643	413.9487	0.0000	0.0000	4373.4973

[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].