SACADA Database Code: 689

Topology: 4^4T61-CA

# of independent nodes (IN): 4
Transitivity: [4(10)62]
Space Group: P21/c
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
4^4T61-CA (SACADA #689)		3.445		0.528	404.5	433.0	80.1	SACADA[1]
4^4T61-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

7907.8537	1037.6843	1456.1799	0.0000	-0.0000	445.8421
1037.6843	10345.6197	811.9030	-0.0000	0.0000	-112.3819
1456.1799	811.9030	11976.4288	-0.0000	-0.0000	-199.5745
0.0000	-0.0000	-0.0000	3256.7441	-178.0780	0.0000
-0.0000	0.0000	-0.0000	-178.0780	4895.5708	0.0000
445.8421	-112.3819	-199.5745	0.0000	-0.0000	4930.6472

[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].