SACADA Database Code: 692

Topology: 4^4T65-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(10)4]
Space Group: P2/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
4^4T65-CA (SACADA #692)		3.327		0.489	383.8	388.4	70.2	SACADA[1]
4^4T65-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9336.0511	1297.8707	1215.7712	0.0000	-0.0000	437.6511
1297.8707	8943.1423	417.3799	0.0000	0.0000	-195.9331
1215.7712	417.3799	10461.3862	0.0000	-0.0000	116.3800
0.0000	-0.0000	-0.0000	3106.4760	-9.8460	-0.0000
-0.0000	0.0000	0.0000	-9.8460	3211.1558	0.0000
437.6511	-195.9331	116.3800	-0.0000	0.0000	4837.2641

[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].