SACADA Database Code: 649

Topology: 4^4T15-CA

# of independent nodes (IN): 4
Transitivity: [4(10)84]
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
4^4T15-CA (SACADA #649)		3.494		0.429	419.8	476.1	89.5	SACADA[1]
4^4T15-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10782.8906	651.5664	836.2842	-0.0000	0.0000	369.1183
651.5664	12425.0703	504.4524	0.0000	0.0000	-56.3506
836.2842	504.4524	10653.1466	0.0000	0.0000	11.4423
-0.0000	-0.0000	0.0000	5056.9855	-130.0266	-0.0000
-0.0000	0.0000	0.0000	-130.0266	4416.1192	0.0000
369.1183	-56.3506	11.4423	-0.0000	0.0000	3906.5687

[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].