SACADA Database Code: 662

Topology: 4^4T28-CA

# of independent nodes (IN): 4
Transitivity: [4973]
Space Group: Ima2
Pearson: oI32
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
4^4T28-CA (SACADA #662)		3.170		0.372	379.2	347.5	58.5	SACADA[1]
4^4T28-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

9422.9484	1454.4823	623.9079	-0.0000	-0.0000	0.0000
1454.4823	8097.7012	1252.9071	0.0000	0.0000	0.0000
623.9079	1252.9071	9988.2140	-0.0000	0.0000	-0.0000
-0.0000	0.0000	-0.0000	2294.6354	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	4563.9171	0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	3045.1712

[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].