SACADA Database Code: 656

Topology: 4^4T21-CA

# of independent nodes (IN): 4
Transitivity: [4962]
Space Group: Pbca
Pearson: oP32
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
4^4T21-CA (SACADA #656)		3.435		0.224	410.2	481.9	91.1	SACADA[1]
4^4T21-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10317.4744	703.9614	176.0910	-0.0000	0.0000	0.0000
703.9614	11427.8642	879.7103	0.0000	-0.0000	0.0000
176.0910	879.7103	11753.8969	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	4413.6754	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	5134.1387	-0.0000
0.0000	0.0000	0.0000	-0.0000	-0.0000	4113.6041

[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].