SACADA Database Code: 701

Topology: 4^4T8-CA

# of independent nodes (IN): 4
Transitivity: [4994]
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
4^4T8-CA (SACADA #701)		3.532		0.302	437.4	503.5	94.9	SACADA[1]
4^4T8-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

12627.7958	811.2328	759.2533	0.0000	0.0000	49.9824
811.2328	11136.2610	769.7826	0.0000	0.0000	73.8177
759.2533	769.7826	10995.2247	0.0000	-0.0000	-194.3269
0.0000	0.0000	-0.0000	5226.3699	-12.3777	0.0000
0.0000	0.0000	-0.0000	-12.3777	4151.4918	-0.0000
49.9824	73.8177	-194.3269	0.0000	-0.0000	5132.9204

[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].