SACADA Database Code: 653

Topology: 4^4T19-CA

# of independent nodes (IN): 4
Transitivity: [4(11)(11)5]
Space Group: Pnma
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
4^4T19-CA (SACADA #653)		3.351		0.214	409.1	435.5	80.4	SACADA[1]
4^4T19-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10943.7836	424.2675	1674.3673	0.0000	0.0000	0.0000
424.2675	11026.7547	745.2823	0.0000	0.0000	-0.0000
1674.3673	745.2823	9223.7510	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	4271.6766	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	3615.5527	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	4628.6204

[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].