SACADA Database Code: 651

Topology: 4^4T17-CA

# of independent nodes (IN): 4
Transitivity: [4852]
Space Group: Pnma
Pearson: oP24
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
4^4T17-CA (SACADA #651)		3.406		0.221	418.8	483.9	91.3	SACADA[1]
4^4T17-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10687.0500	525.5802	342.0364	0.0000	-0.0000	-0.0000
525.5802	12364.3903	574.6798	-0.0000	-0.0000	0.0000
342.0364	574.6798	11839.0842	-0.0000	0.0000	-0.0000
-0.0000	0.0000	-0.0000	4385.7468	-0.0000	-0.0000
-0.0000	0.0000	0.0000	-0.0000	4781.4466	0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	4083.8887

[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].