SACADA Database Code: 685

Topology: 4^4T57-CA

# of independent nodes (IN): 4
Transitivity: [4(11)63]
Space Group: C2/c
Pearson: mS32
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
4^4T57-CA (SACADA #685)		3.398		0.459	384.9	438.5	82.5	SACADA[1]
4^4T57-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

10581.3200	528.2487	688.0997	-0.0000	-0.0000	159.3142
528.2487	8636.6280	1738.9042	0.0000	-0.0000	284.1072
688.0997	1738.9042	9557.6329	-0.0000	-0.0000	-84.4672
0.0000	-0.0000	-0.0000	3938.3260	26.3700	0.0000
-0.0000	0.0000	0.0000	26.3700	5145.5234	0.0000
159.3142	284.1072	-84.4672	0.0000	-0.0000	4420.3931

[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].