

SACADA Database Code: 536

Topology: 4²T36-CA

of independent nodes (IN): 2

Transitivity: [2773]

Space Group: I41/amd

Pearson: tI64

Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ² T36-CA (SACADA #536)		3.056		1.128	294.8	260.7	42.2	SACADA ¹
4 ² T36-CA								doi: 10.1038/s41524-021-00491-y ✉

Elasticity tensor (kBar)¹

5948.0478	1708.1278	1123.6428	0.0000	0.0000	0.0000
1708.1278	5948.0478	1123.6428	0.0000	-0.0000	0.0000
1123.6428	1123.6428	6722.0825	-0.0000	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	3242.3637	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	2515.1963	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	2515.1963

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].