

SACADA Database Code: 596

Topology: 4³T172-CA

of independent nodes (IN): 3
Transitivity: [3(10)(10)4]
Space Group: P42/nmc
Pearson: tP48
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 ³ T172-CA (SACADA #596)		2.972		0.694	306.1	242.1	33.5	SACADA ¹
4 ³ T172-CA								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

5550.0676	1305.2179	1398.4211	-0.0000	0.0000	0.0000
1305.2179	5550.0676	1398.4211	0.0000	0.0000	0.0000
1398.4211	1398.4211	8854.7592	0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	1942.5688	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	2545.1226	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	2545.1226

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].