

SACADA Database Code: 590

Topology: 4³T166-CA

of independent nodes (IN): 3
Transitivity: [3794]
Space Group: P42/mmc
Pearson: tP32
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 T166-CA (SACADA #590)		2.238		1.459	131.8	69.9	8.8	SACADA ¹
4 ³ T166-CA								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

1434.2958	471.9365	1355.2055	0.0000	-0.0000	0.0000
471.9365	1434.2958	1355.2055	0.0000	-0.0000	0.0000
1355.2055	1355.2055	6229.9996	-0.0000	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	303.3108	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	934.8517	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	-0.0000	934.8517

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].