

SACADA Database Code: 600

Topology: 4³T176-CA

of independent nodes (IN): 3
Transitivity: [37(10)7]
Space Group: I4/mmm
Pearson: tI48
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 T176-CA (SACADA #600)		3.185		0.441	373.0	343.8	58.1	SACADA ¹
4 ³ T176-CA								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

7611.5297	1580.0529	1216.7369	0.0000	0.0000	0.0000
1580.0529	7611.5297	1216.7369	0.0000	0.0000	0.0000
1216.7369	1216.7369	10583.7304	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	2828.0074	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	3650.5149	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	3650.5148

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].