

SACADA Database Code: 547

Topology: 4²T285

of independent nodes (IN): 2
Transitivity: [2553]
Space Group: Pbcn
Pearson: oP16
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 T285 (SACADA #547)		3.474		0.471	408.3	450.4	84.1	SACADA ¹
4 ² T285								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

9280.1227	858.3629	1152.5939	-0.0000	0.0000	-0.0000
858.3629	9793.5072	1213.7120	-0.0000	0.0000	-0.0000
1152.5939	1213.7120	11399.5226	-0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	3302.1141	-0.0000	-0.0000
0.0000	0.0000	-0.0000	-0.0000	5115.3259	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	5371.5072

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].