

SACADA Database Code: 570

Topology: 4³T142

of independent nodes (IN): 3
Transitivity: [3973]
Space Group: C2/m
Pearson: mS24
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 T142 (SACADA #570)		3.358		0.217	415.1	427.3	77.8	SACADA ¹
4 ³ T142								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

9763.9231	1541.3235	1099.2358	-0.0000	0.0000	-111.1434
1541.3235	9481.6235	834.0869	-0.0000	-0.0000	170.5688
1099.2358	834.0869	11211.0620	0.0000	0.0000	-275.2915
-0.0000	0.0000	0.0000	3390.9274	-203.4091	0.0000
0.0000	-0.0000	0.0000	-203.4091	4304.5785	0.0000
-111.1434	170.5688	-275.2915	0.0000	-0.0000	4886.3752

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].