

SACADA Database Code: 573

Topology: 4³T148-CA

of independent nodes (IN): 3
Transitivity: [3762]
Space Group: I2/a
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 T148-CA (SACADA #573)		3.235		0.309	388.9	392.6	70.8	SACADA ¹
4 ³ T148-CA								doi: 10.1038/s41524-021-00491-y ↗

Elasticity tensor (kBar)¹

9120.7501	1319.2633	878.8401	-0.0000	-0.0000	-17.4684
1319.2633	9302.5585	1665.5065	-0.0000	0.0000	-409.9047
878.8401	1665.5065	8885.8455	-0.0000	-0.0000	-186.3363
-0.0000	-0.0000	-0.0000	4186.4703	-27.8613	-0.0000
-0.0000	0.0000	-0.0000	-27.8613	3798.0807	-0.0000
-17.4684	-409.9047	-186.3363	0.0000	-0.0000	3858.4677

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].