

SACADA Database Code: 562

Topology: 4³T59-CA

of independent nodes (IN): 3
Transitivity: [3741]
Space Group: P21/c
Pearson: mP12
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 T59-CA (SACADA #562)		3.418		0.451	391.7	439.4	82.4	SACADA ¹
4 ³ T59-CA								doi: 10.1038/s41524-021-00491-y ✉

Elasticity tensor (kBar)¹

8347.1825	955.7229	1576.9748	-0.0000	-0.0000	443.9638
955.7229	10405.4473	737.0603	-0.0000	-0.0000	46.2798
1576.9748	737.0603	10045.4559	0.0000	-0.0000	-872.3914
-0.0000	-0.0000	0.0000	4738.8088	-24.3839	0.0000
-0.0000	-0.0000	-0.0000	-24.3839	4281.7641	0.0000
443.9638	46.2798	-872.3914	0.0000	0.0000	4542.7464

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].