

SACADA Database Code: 645

Topology: 4⁴T11-CA

of independent nodes (IN): 4
Transitivity: [4(10)84]
Space Group: P21/c
Pearson: mP16
Coordination Number (CN): 4

Year: 2023

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁴ T11-CA (SACADA #645)		3.506		0.447	424.7	480.8	90.3	SACADA ¹
4 ⁴ T11-CA								doi: 10.1107/S205252062300255X 📄

Elasticity tensor (kBar)¹

11238.3095	724.4453	833.7480	-0.0000	0.0000	-83.0246
724.4453	12571.6173	504.8125	0.0000	-0.0000	-6.4104
833.7480	504.8125	10387.8298	-0.0000	-0.0000	-359.6336
-0.0000	0.0000	0.0000	5174.2273	-315.0926	-0.0000
0.0000	-0.0000	-0.0000	-315.0926	4359.9405	0.0000
-83.0246	-6.4104	-359.6336	-0.0000	0.0000	3999.9444

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].