

SACADA Database Code: 648

Topology: 4⁴T14-CA

of independent nodes (IN): 4
Transitivity: [4964]
Space Group: C2/m
Pearson: mS24
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 T14-CA (SACADA #648)		3.400		0.223	418.9	483.1	91.1	SACADA ¹
4 ⁴ T14-CA								doi: 10.1107/S205252062300255X 📄

Elasticity tensor (kBar)¹

10505.0348	520.9296	1425.6821	-0.0000	-0.0000	-952.4365
520.9296	12350.7148	595.5480	0.0000	0.0000	-49.0329
1425.6821	595.5480	9818.2355	0.0000	0.0000	319.8743
-0.0000	0.0000	0.0000	4551.2555	-257.8837	-0.0000
-0.0000	0.0000	0.0000	-257.8837	4560.7895	-0.0000
-952.4365	-49.0329	319.8743	-0.0000	-0.0000	5125.7466

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].