

SACADA Database Code: 631

Topology: 4²T46-CA

of independent nodes (IN): 2
Transitivity: [2663]
Space Group: C2221
Pearson: oS16
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 ² T46-CA (SACADA #631)		3.487		0.501	417.2	484.5	91.5	SACADA ¹
4 ² T46-CA								doi: 10.1107/S205252062300255X 📄

Elasticity tensor (kBar)¹

10663.3252	222.6915	1270.5419	0.0000	0.0000	0.0000
222.6915	12357.6234	204.5934	-0.0000	-0.0000	0.0000
1270.5419	204.5934	11142.9031	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	4136.1425	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	4643.3211	-0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	4803.0197

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].