

SACADA Database Code: 642

Topology: 4³T205-CA

of independent nodes (IN): 3
Transitivity: [3663]
Space Group: P2221
Pearson: oP8
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 ³ T205-CA (SACADA #642)		3.397		0.836	364.0	343.4	59.3	SACADA ¹
4 ³ T205-CA								doi: 10.1107/S205252062300255X ↗

Elasticity tensor (kBar)¹

8520.2203	573.1205	1573.5349	-0.0000	0.0000	-0.0000
573.1205	11951.2711	1128.2150	0.0000	-0.0000	-0.0000
1573.5349	1128.2150	6389.1935	-0.0000	-0.0000	-0.0000
-0.0000	0.0000	0.0000	4231.4267	-0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	4445.1852	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	1840.1060

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].