

SACADA Database Code: 229

Topology: 4⁴T105

of independent nodes (IN): 4
Transitivity: [4974]
Space Group: P-421c
Pearson: tP32
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁴ T105 (SACADA #229)		3.595		0.793	389.9	492.4	94.0	SACADA ¹
t32		3.530	5.41		352			doi: 10.1103/PhysRevB.94.174102 ↗

Elasticity tensor (kBar)¹

10375.2332	510.1194	759.5629	0.0000	-0.0000	-0.0000
510.1194	10375.2332	759.5629	-0.0000	-0.0000	-0.0000
759.5629	759.5629	10278.7045	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	4852.8270	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	5051.5368	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	5051.5368

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].