

SACADA Database Code: 331

Topology: 4¹³T4

of independent nodes (IN): 13
Transitivity: [(13)(17)(17)(13)]
Space Group: Imma
Pearson: oI72
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 ¹³ T4 (SACADA #331)		3.504		0.608	422.0	494.2	93.4	SACADA ¹
8(II)								doi: 10.1103/PhysRevB.93.085201 □

Elasticity tensor (kBar)¹

11264.6444	280.4987	1214.0139	0.0000	0.0000	0.0000
280.4987	10898.9790	1260.4273	0.0000	0.0000	-0.0000
1214.0139	1260.4273	10313.8880	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	4353.2111	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	5156.7328	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	5394.5658

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].