

SACADA Database Code: 316

Topology: $4^{10}T5$

of independent nodes (IN): 10

Transitivity: [(10)(19)(14)4]

Space Group: P42/nmc

Pearson: tP106

Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$4^{10}T5$ (SACADA #316)		2.979		0.948	301.8	335.5	62.8	SACADA ¹
KX		2.94	2.01		302.7		79.9	doi: 10.1063/1.4802002 

Elasticity tensor (kBar)¹

6608.7763	1011.2678	907.4922	-0.0000	-0.0000	-0.0000
1011.2678	6608.7763	907.4922	0.0000	-0.0000	0.0000
907.4922	907.4922	8438.5147	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	3364.0859	0.0000	0.0000
-0.0000	-0.0000	0.0000	0.0000	3614.1326	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	-0.0000	3614.1326

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].