

SACADA Database Code: 328

Topology: 4¹²T5

of independent nodes (IN): 12
Transitivity: [(12)(20)(19)(11)]
Space Group: P2/m
Pearson: mP24
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ¹² T5 (SACADA #328)		3.477		0.718	408.5	479.1	90.6	SACADA ¹
S-S1A4	10.6							doi: 10.1103/PhysRevLett.108.135501 [4]

Elasticity tensor (kBar)¹

11553.9234	986.6694	545.2484	0.0000	-0.0000	254.7832
986.6694	11400.5617	158.9269	-0.0000	0.0000	117.3928
545.2484	158.9269	10511.4429	0.0000	0.0000	-254.5795
0.0000	-0.0000	0.0000	5291.7666	189.9412	0.0000
-0.0000	0.0000	0.0000	189.9412	3943.8756	-0.0000
254.7832	117.3928	-254.5795	0.0000	-0.0000	4328.8932

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].