

SACADA Database Code: 450

Topology: 4¹⁰T11

of independent nodes (IN): 10
Transitivity: [(10)(20)(11)1]
Space Group: P1
Pearson: aP10
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ¹⁰ T11 (SACADA #450)		3.284		0.793	386.6	406.4	74.7	SACADA ¹
G157								doi: 10.1002/cphc.201700151 cf

Elasticity tensor (kBar)¹

8486.8923	1630.9266	1040.0839	-53.9078	-81.9744	-50.2309
1630.9266	8532.7294	1283.1333	-76.9259	96.3215	69.1834
1040.0839	1283.1333	9915.1964	60.6464	252.2004	-95.3643
-53.9078	-76.9259	60.6464	4318.8916	-104.8582	-4.2246
-81.9744	96.3215	252.2004	-104.8582	3872.4015	-177.4240
-50.2309	69.1834	-95.3643	-4.2246	-177.4240	4584.0502

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].