

## SACADA Database Code: 550

Topology: 4<sup>3</sup>T31-CA

# of independent nodes (IN): 3

Transitivity: [3983]

Space Group: Cmcm

Pearson: oS40

Coordination Number (CN): 4

Year: 2021

## Data

Name	Pressure, GPa	Density, g/cm <sup>3</sup>	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 <sup>3</sup> T31-CA (SACADA #550)		3.395		0.190	419.9	446.5	82.4	SACADA <sup>1</sup>
4 <sup>3</sup> T31-CA								doi: <a href="https://doi.org/10.1038/s41524-021-00491-y">10.1038/s41524-021-00491-y</a>

### Elasticity tensor (kBar)<sup>1</sup>

10432.5510	1147.3451	1124.0113	0.0000	-0.0000	0.0000
1147.3451	11455.8969	651.0479	0.0000	0.0000	-0.0000
1124.0113	651.0479	10101.6510	-0.0000	-0.0000	-0.0000
0.0000	0.0000	-0.0000	4989.2416	0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	4321.7683	-0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	3528.5836

<sup>1</sup> 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  $\Gamma$ -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  $\nu$  — 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].