

## SACADA Database Code: 135

Topology: 4<sup>2</sup>T109

# of independent nodes (IN): 2

Transitivity: [2543]

Space Group: C2

Pearson: mS8

Coordination Number (CN): 4

Year: 2004

## 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>2</sup> T109 (SACADA #135)		2.962		1.922	228.6	219.8	38.5	SACADA <sup>1</sup>
I		2.865	0.9		154.0			doi: <a href="https://doi.org/10.1103/PhysRevB.70.045101">10.1103/PhysRevB.70.045101</a> †

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

2864.4869	423.2384	1029.4305	0.0000	-0.0000	357.8953
423.2384	5362.3591	1751.4662	-0.0000	-0.0000	34.1083
1029.4305	1751.4662	8701.4748	-0.0000	-0.0000	1365.5557
0.0000	-0.0000	-0.0000	1752.8148	4.9789	-0.0000
-0.0000	-0.0000	-0.0000	4.9789	2855.7325	0.0000
357.8953	34.1083	1365.5557	-0.0000	0.0000	2355.4383

<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].