## **SACADA Database Code: 120**

Topology: ggl a

# of independent nodes (IN): 2

Transitivity: [2343] Space Group: R-3c Pearson: hR54

Coordination Number (CN): 3, 4 (2:1)

Year: 2017

## **Data**

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ggl (SACADA #120)		1.835		0.807	196.2	65.7	9.9	SACADA <sup>1</sup>
ggl								doi: 10.1007/s11224-016-0782-1 ថា

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

2373.5411	1953.0001	1048.6907	-0.0000	-65.9682	0.0000
1953.0001	2373.5411	1048.6907	-0.0000	65.9682	-0.0000
1048.6907	1048.6907	5146.8256	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	210.2705	-0.0000	-65.9682
-65.9682	65.9682	-0.0000	-0.0000	1164.1364	-0.0000
0.0000	-0.0000	0.0000	-65.9682	-0.0000	1164.1364

<sup>&</sup>lt;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  $2\pi \times 0.025~\text{Å}^{-1}$  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  $\text{Å}^{-1}$  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  $H_{\nu}$  has been estimated according to Oganov's model [9].