SACADA Database Code: 120

Topology: ggl

# 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[1]
ggl								doi: 10.1007/s11224-016-0782-1

Elasticity tensor (kBar)[1]

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

[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 $2\pi \times 0.025$ 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 Å^{-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].