

SACADA Database Code: 102

Topology: [isq](#) 

of independent nodes (IN): 2
Transitivity: [2331]
Space Group: P42/mnm
Pearson: tP12
Coordination Number (CN): 4

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
isq (SACADA #102)		3.099		0.245	372.5	374.5	67.4	SACADA ¹
P42/mnm			4.55		362.6			doi: 10.1103/PhysRevB.89.184112 

Elasticity tensor (kBar)¹

8072.7883	1087.2396	1607.4622	-0.0000	-0.0000	0.0000
1087.2396	8072.7883	1607.4622	-0.0000	0.0000	0.0000
1607.4622	1607.4622	8864.2600	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	4655.3463	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	3649.4482	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	3649.4483

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].