

SACADA Database Code: 82

Topology: [pcl](#) 

of independent nodes (IN): 1
Transitivity: [1441]
Space Group: Cmc_m
Pearson: oS16
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcl (SACADA #82)		3.041		0.445	357.1	292.4	42.6	SACADA ¹
LA7								doi: 10.1134/s1063776111060173 
LA7								link 

Elasticity tensor (kBar)¹

8097.7294	2860.0136	826.5518	0.0000	-0.0000	0.0000
2860.0136	4868.0367	1779.6158	-0.0000	0.0000	0.0000
826.5518	1779.6158	8711.7592	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	3516.9350	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	2819.7572	0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	3812.0270

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 $10^{-5} \text{ eV \AA}^{-1}$ 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].

