

SACADA Database Code: 73

Topology: [mon](#) 

of independent nodes (IN): 1
Transitivity: [1342]
Space Group: I41/amd
Pearson: tI16
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
mon (SACADA #73)		2.970		0.499	349.1	314.5	52.0	SACADA ¹
LA10		2.904						doi: 10.1134/s1063776114060090 

Elasticity tensor (kBar)¹

10085.1157	269.9251	477.6526	-0.0000	-0.0000	-0.0000
269.9251	10085.1157	477.6526	0.0000	-0.0000	-0.0000
477.6526	477.6526	8838.4618	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	1564.1009	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	3067.5245	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	0.0000	3067.5243

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].