SACADA Database Code: 128

Topology: lon-a

# of independent nodes (IN): 2
Transitivity: [2443]
Space Group: P63/mmc
Pearson: hP16
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
lon-a (SACADA #128)		1.515		1.859	162.4	46.5	7.2	SACADA[1]
L-carbon		1.50			158.1			doi: 10.1073/pnas.1311028110

Elasticity tensor (kBar)[1]

2393.7808	1392.6718	1134.3988	0.0000	-0.0000	-0.0000
1392.6718	2393.7808	1134.3988	0.0000	0.0000	0.0000
1134.3988	1134.3988	2510.4012	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	500.5545	0.0000	-0.0000
-0.0000	0.0000	0.0000	0.0000	346.6482	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	346.6481

[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].