SACADA Database Code: 38

Topology: lon (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1222]
Space Group: P-6m2
Pearson: hP6
Coordination Number (CN): 2, 4 (1:1)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
lon (SACADA #38)		3.011		1.343	306.0	152.3	19.8	SACADA[1]
2HYD		3.1	Semicond		320.3	191.8	59.2	doi: 10.1016/j.diamond.2014.04.005

Elasticity tensor (kBar)[1]

6479.2918	738.8703	131.3216	0.0000	-0.0000	-0.0000
738.8703	6479.2918	131.3216	-0.0000	-0.0000	0.0000
131.3216	131.3216	13932.5752	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	2870.2108	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	285.2748	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	285.2748

[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].