SACADA Database Code: 13

Topology: lcs

# of independent nodes (IN): 1
Transitivity: [1121]
Space Group: Ia-3d
Pearson: cI24
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
lcs (SACADA #13)		3.512		1.447	427.2	457.4	84.6	SACADA[1]
lcs								doi: 10.1524/zkri.2013.1620
iceII-carbon		3.46	1.92		406.1			doi: 10.1021/jp5080048
BC12		3.461	2.98		393			doi: 10.1103/PhysRevB.91.214106
BC12		3.461			441	451	65.65	doi: 10.1088/0953-8984/28/47/475402
BC12		3.461			393			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

10843.8686	985.7520	985.7520	-0.0000	0.0000	-0.0000
985.7520	10843.8686	985.7520	0.0000	0.0000	0.0000
985.7520	985.7520	10843.8686	-0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	4349.6297	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	4349.6297	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	4349.6297

[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].