SACADA Database Code: 123

Topology: xcb

# of independent nodes (IN): 2
Transitivity: [2432]
Space Group: P63/mmc
Pearson: hP16
Coordination Number (CN): 3, 4 (3:1)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
xcb (SACADA #123)		1.859		0.828	205.2	103.8	13.4	SACADA[1]
3D-(9,0)		1.902			207.7	101.5	36.0	doi: 10.1021/nn202053t
hP16-carbon			Metal		207.5	103.4	11.1	doi: 10.3103/s1063457614040042
hP16-carbon								doi: 10.1002/pssb.201552234

Elasticity tensor (kBar)[1]

2507.8109	1913.8458	748.8732	0.0000	0.0000	-0.0000
1913.8458	2507.8109	748.8732	0.0000	-0.0000	0.0000
748.8732	748.8732	7527.0521	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	296.9826	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	1988.4777	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	1988.4777

[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].