SACADA Database Code: 224

Topology: cbn

# of independent nodes (IN): 4
Transitivity: [4863]
Space Group: C2/m
Pearson: mS16
Coordination Number (CN): 4

Year: 2006

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cbn (SACADA #224)		3.388		0.734	418.9	461.6	86.1	SACADA[1]
5+7								doi: 10.1063/1.2210932
M-carbon					431.2		83.1	doi: 10.1103/PhysRevLett.102.175506
M-carbon								doi: 10.1209/0295-5075/87/56003
M-carbon								doi: 10.1063/1.3610996
M-carbon								link
M-carbon								doi: 10.1103/PhysRevB.84.092103
M-carbon								doi: 10.1103/PhysRevB.83.155452
M-carbon								doi: 10.1021/ja304380p
M-carbon								link
M-carbon								doi: 10.1103/PhysRevB.85.144115
M-carbon								doi: 10.1103/PhysRevB.85.155428
M-carbon								doi: 10.1016/j.ssc.2012.05.022
M-carbon								doi: 10.1038/srep00471
M-carbon								link
M-carbon		3.45						doi: 10.3103/s1063457613010012
M-12								doi: 10.1103/PhysRevB.88.014102
M-carbon					414			doi: 10.1016/j.carbon.2014.06.050
M-carbon								doi: 10.1088/0253-6102/64/2/237
M-carbon								doi: 10.1007/s10853-015-9266-8

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
M-carbon								doi: 10.1142/s0217984915300112
M-carbon								doi: 10.1103/PhysRevB.93.085201
M-carbon								doi: 10.1039/c6ra02081j

Elasticity tensor (kBar)[1]

9294.7778	598.5293	1780.7077	0.0000	-0.0000	434.8265
598.5293	11171.8554	872.5110	-0.0000	0.0000	-355.8726
1780.7077	872.5110	10821.7007	-0.0000	0.0000	330.4730
0.0000	-0.0000	-0.0000	3933.5656	-273.4393	0.0000
-0.0000	0.0000	0.0000	-273.4393	5301.0061	-0.0000
434.8265	-355.8726	330.4730	0.0000	-0.0000	4685.0266

[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].