SACADA Database Code: 218

Topology: cnw

# of independent nodes (IN): 4
Transitivity: [4753]
Space Group: Pnma
Pearson: oP16
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cnw (SACADA #218)		3.398		0.725	417.8	459.4	85.7	SACADA[1]
W-carbon								doi: 10.1103/PhysRevLett.106.075501
W-carbon								doi: 10.1063/1.3610996
W-carbon			4.39		444.5			doi: 10.1021/ja304380p
W-carbon					403	451	78.5	doi: 10.1103/PhysRevB.85.144115
W-carbon			3.45-3.35		468-447			doi: 10.1103/PhysRevB.85.155428
W-carbon							83.1	doi: 10.1016/j.ssc.2012.05.022
W-carbon								doi: 10.1038/srep00471
W-carbon								link
W-carbon					431.4		93.8	doi: 10.3103/s1063457613010012
W-carbon					432			doi: 10.1016/j.carbon.2014.06.050
W-carbon								doi: 10.1088/0253-6102/64/2/237
W-carbon								doi: 10.1142/s0217984915300112
W-carbon								doi: 10.1103/PhysRevB.93.085201
W-carbon		3.352						doi: 10.1088/0953-8984/28/47/475402

Elasticity tensor (kBar)[1]

9139.4515	551.0633	1834.2876	0.0000	-0.0000	0.0000
551.0633	11147.9595	991.0235	-0.0000	0.0000	0.0000
1834.2876	991.0235	10688.1376	-0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	3904.8679	0.0000	-0.0000
-0.0000	0.0000	0.0000	0.0000	5356.6325	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	4709.6361

[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].