SACADA Database Code: 213

Topology: znp

# of independent nodes (IN): 4
Transitivity: [4664]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
znp (SACADA #213)		3.438		0.659	426.4	470.8	87.9	SACADA[1]
S-carbon		3.399	4.342		468.45			doi: 10.1016/j.ssc.2012.05.022
C-carbon								doi: 10.1021/ja304380p
S-carbon		3.401	4.342		416.23		79.55	doi: 10.3103/s1063457612060123
C-carbon			4.38		427.8			doi: 10.1039/c2cp24066a
S-carbon								doi: 10.3103/s1063457613010012
12B								doi: 10.1103/PhysRevB.88.014102
C-carbon					491			doi: 10.1016/j.carbon.2014.06.050
S-carbon								doi: 10.1088/0256-307x/32/9/096201
C-carbon								doi: 10.1142/s0217984915300112
S-carbon								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11398.4152	1085.1136	371.3694	-0.0000	0.0000	-0.0000
1085.1136	9964.8536	1729.9441	-0.0000	0.0000	-0.0000
371.3694	1729.9441	10644.3830	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	5124.6197	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	4773.9999	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	4159.4667

[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].