SACADA Database Code: 225

Topology: 4^4T35

# of independent nodes (IN): 4
Transitivity: [4873]
Space Group: P2/m
Pearson: mP8
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
4^4T35 (SACADA #225)		3.377		0.737	414.0	452.1	84.1	SACADA[1]
F-carbon								doi: 10.1021/ja304380p
F-carbon			4.52		410.2	460.5	93.9	doi: 10.1088/0953-8984/24/16/165504
Z-carbon-1			4.54		429		66.7	doi: 10.1021/ja301582d
J-carbon			4.56		394.9			doi: 10.1063/1.4732538
S-carbon		3.44	5.52		412.6	457.7	78.3	doi: 10.1103/PhysRevLett.108.135501
M10-carbon			4.4		423.7		93.5	doi: 10.1140/epjb/e2013-40639-4
F-carbon					404			doi: 10.1016/j.carbon.2014.06.050
F-carbon								doi: 10.1088/0256-307x/32/9/096201
S-carbon								doi: 10.1142/s0217984915300112
F-C								doi: 10.1016/j.physleta.2015.06.037
F-carbon								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

9891.7384	349.5825	1361.4849	-0.0000	0.0000	52.3127
349.5825	11112.0755	1141.1675	0.0000	0.0000	89.3936
1361.4849	1141.1675	10612.4620	0.0000	0.0000	-91.0072
-0.0000	0.0000	0.0000	3712.5176	147.8727	-0.0000
0.0000	0.0000	0.0000	147.8727	5091.8289	0.0000
52.3127	89.3936	-91.0072	-0.0000	0.0000	4382.3362

[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].