SACADA Database Code: 221

Topology: 4^4T33

# of independent nodes (IN): 4
Transitivity: [4763]
Space Group: Pbam
Pearson: oP16
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
4^4T33 (SACADA #221)		3.392		0.711	416.6	450.5	83.6	SACADA[1]
H-carbon		3.339	4.459		445.88			doi: 10.1016/j.ssc.2012.05.022
O-carbon								doi: 10.1021/ja304380p
H-carbon		3.341	4.459		400.94		76.92	doi: 10.3103/s1063457612060123
R carbon		3.45	5.51		434.2	462.4	75.0	doi: 10.1103/PhysRevLett.108.135501
O-carbon			4.54		438.6			doi: 10.1103/PhysRevB.85.033410
H-carbon								doi: 10.3103/s1063457613010012
O-carbon					430			doi: 10.1016/j.carbon.2014.06.050
O-carbon								doi: 10.1142/s0217984915300112
R carbon								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

9944.1362	1770.7597	965.0973	-0.0000	-0.0000	0.0000
1770.7597	10036.5579	421.8222	0.0000	-0.0000	0.0000
965.0973	421.8222	11205.6218	-0.0000	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	4483.6283	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	-0.0000	3889.5765	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	4954.5530

[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].