SACADA Database Code: 101

Topology: tfh

# of independent nodes (IN): 2
Transitivity: [2322]
Space Group: Im-3
Pearson: cI40
Coordination Number (CN): 3, 4 (1:1)

Year: 2010

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
tfh (SACADA #101)		2.420		1.234	203.9	153.2	19.6	SACADA[1]
bcc-C20								doi: 10.3103/s1063457610020012
bcc-C20		2.47	2.26		200.06	156.94		doi: 10.1021/jp3064323

Elasticity tensor (kBar)[1]

3812.0570	1151.6302	1151.6302	0.0000	0.0000	-0.0000
1151.6302	3812.0570	1151.6302	0.0000	-0.0000	-0.0000
1151.6302	1151.6302	3812.0570	-0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	1685.0873	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	1685.0873	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	1685.0873

[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].