SACADA Database Code: 107

Topology: cdp

# of independent nodes (IN): 2
Transitivity: [2332]
Space Group: P42/ncm
Pearson: tP12
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
cdp (SACADA #107)		3.393		0.683	420.0	465.3	86.9	SACADA[1]
T12			3.59		424.8	479.3	94.0	doi: 10.1021/ja304380p
T12		3.342			403.2			doi: 10.1073/pnas.1311028110
cdp								doi: 10.1524/zkri.2013.1620
T12					434			doi: 10.1016/j.carbon.2014.06.050
P42/ncm					403			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

9614.3876	1812.0544	1356.8280	0.0000	-0.0000	-0.0000
1812.0544	9614.3876	1356.8280	-0.0000	0.0000	0.0000
1356.8280	1356.8280	9530.0788	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	5699.5746	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	4846.2786	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	4846.2785

[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].