SACADA Database Code: 266

Topology: $3^3,4^3$T28

# of independent nodes (IN): 6
Transitivity: [6(12)93]
Space Group: P2/m
Pearson: mP20
Coordination Number (CN): 3, 4 (1:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^3,4^3$T28 (SACADA #266)		2.357		1.414	154.6	118.2	15.5	SACADA[1]
phaseI	0-100	2.34	2.7		186			doi: 10.1016/j.carbon.2013.06.086

Elasticity tensor (kBar)[1]

4576.2643	258.9882	1025.3222	0.0000	-0.0000	-870.8466
258.9882	4543.7337	238.9578	-0.0000	0.0000	-137.1344
1025.3222	238.9578	2331.6641	0.0000	0.0000	-583.3071
0.0000	0.0000	0.0000	1109.9875	-251.1220	0.0000
0.0000	0.0000	0.0000	-251.1220	762.5036	-0.0000
-870.8466	-137.1344	-583.3071	0.0000	-0.0000	1125.6364

[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].