SACADA Database Code: 286

Topology: 3^6,4T10

# of independent nodes (IN): 7
Transitivity: -
Space Group: P6/mmm
Pearson: hP52
Coordination Number (CN): 3, 4 (12:1)

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^6,4T10 (SACADA #286)		.810		0.671	-	-	-	SACADA[1]
honeycomb foam		0.80	Metal		72			doi: 10.1039/C0CC05738J

Elasticity tensor (kBar)[1]

838.4069	957.2981	304.1506	-35.3867	2.1024	1.5322
957.2981	1009.7665	313.2617	-34.7513	-3.0123	-1.2131
304.1506	313.2617	3741.3894	-8.4201	0.7304	-0.5667
-35.3867	-34.7513	-8.4201	-19.7054	0.1359	-1.9448
2.1024	-3.0123	0.7304	0.1359	693.9916	-12.2386
1.5322	-1.2131	-0.5667	-1.9448	-12.2386	660.4498

[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].