SACADA Database Code: 287

Topology: $3^2,4^6T12$

# of independent nodes (IN): 8
Transitivity: [8986]
Space Group: Pmma
Pearson: oP16
Coordination Number (CN): 3, 4 (1:3)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^6T12$ (SACADA #287)		3.357		0.701	409.5	365.5	59.9	SACADA[1]
16E	20							doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

12068.1572	128.2157	1662.3060	0.0000	-0.0000	0.0000
128.2157	8029.1084	1532.3385	0.0000	0.0000	-0.0000
1662.3060	1532.3385	10834.3117	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	3158.5179	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	1861.6048	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	5528.0742

[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].