SACADA Database Code: 262

Topology: 4^6T7

# of independent nodes (IN): 6
Transitivity: [6(10)(10)5]
Space Group: C2/m
Pearson: mS24
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
4^6T7 (SACADA #262)		3.446		0.670	426.2	473.5	88.5	SACADA[1]
Z-carbon-3			5.27		443		92.6	doi: 10.1021/ja301582d
12C								doi: 10.1103/PhysRevB.88.014102

Elasticity tensor (kBar)[1]

10041.2702	507.1503	1383.3170	-0.0000	0.0000	218.2427
507.1503	11268.9738	1118.3722	0.0000	-0.0000	-272.1466
1383.3170	1118.3722	11115.0157	-0.0000	0.0000	290.1574
-0.0000	0.0000	-0.0000	4044.8956	-253.4115	-0.0000
0.0000	-0.0000	0.0000	-253.4115	5301.4693	0.0000
218.2427	-272.1466	290.1574	-0.0000	0.0000	4645.9849

[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].

PDF / sacada.info