SACADA Database Code: 293

Topology: 4^8T5

# of independent nodes (IN): 8
Transitivity: [8(14)(13)7]
Space Group: P2/m
Pearson: mP16
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^8T5 (SACADA #293)		3.464		0.660	429.5	486.1	91.3	SACADA[1]
Z-carbon-2			4.41		446		92.4	doi: 10.1063/1.4802002

Elasticity tensor (kBar)[1]

10565.1134	560.5744	1068.5867	-0.0000	-0.0000	-188.7553
560.5744	11392.1366	1060.0905	0.0000	-0.0000	399.5970
1068.5867	1060.0905	11364.2168	-0.0000	0.0000	-279.9225
-0.0000	0.0000	-0.0000	4246.3978	388.6509	0.0000
-0.0000	-0.0000	0.0000	388.6509	5302.0503	-0.0000
-188.7553	399.5970	-279.9225	0.0000	-0.0000	4637.2604

[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].