SACADA Database Code: 295

Topology: 4^8T13

# of independent nodes (IN): 8
Transitivity: [8(14)(13)7]
Space Group: P2/m
Pearson: mP16
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
4^8T13 (SACADA #295)		3.454		0.656	428.1	483.6	90.8	SACADA[1]
S-S1Z2	6.2	3.51			437.2	490.4	82.8	doi: 10.1103/PhysRevLett.108.135501
S-S1Z2								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

10493.8206	1212.3080	1402.6631	-0.0000	0.0000	104.1890
1212.3080	11449.3218	325.7139	-0.0000	0.0000	-151.3390
1402.6631	325.7139	10722.5495	0.0000	-0.0000	-0.2687
-0.0000	-0.0000	0.0000	5320.7020	-194.5365	-0.0000
0.0000	0.0000	-0.0000	-194.5365	4187.4551	-0.0000
104.1890	-151.3390	-0.2687	-0.0000	-0.0000	4880.9817

[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].