SACADA Database Code: 296

Topology: 4^8T12

# 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
4^8T12 (SACADA #296)		3.444		0.752	414.9	472.5	88.9	SACADA[1]
S-S1A2	14.4	3.50			424.1		82.6	doi: 10.1103/PhysRevLett.108.135501

Elasticity tensor (kBar)[1]

11652.4853	1086.5780	829.4682	-0.0000	0.0000	382.3725
1086.5780	11575.5848	227.9577	-0.0000	-0.0000	188.5766
829.4682	227.9577	9990.1370	0.0000	-0.0000	-271.4489
-0.0000	-0.0000	0.0000	5333.6829	318.8334	0.0000
0.0000	-0.0000	-0.0000	318.8334	3818.3647	-0.0000
382.3725	188.5766	-271.4489	0.0000	-0.0000	4337.9409

[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].