SACADA Database Code: 327

Topology: 4^{12}T2

# of independent nodes (IN): 12
Transitivity: [(12)(20)(18)(10)]
Space Group: P2/m
Pearson: mP24
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^{12}T2 (SACADA #327)		3.427		0.683	406.6	461.1	86.6	SACADA[1]
S-S'2Z2	8.3							doi: 10.1103/PhysRevLett.108.135501

Elasticity tensor (kBar)[1]

10170.8177	1075.2650	1313.3124	-0.0000	-0.0000	-61.3601
1075.2650	10988.5523	309.4776	-0.0000	-0.0000	23.8853
1313.3124	309.4776	10064.5750	0.0000	0.0000	90.1952
-0.0000	-0.0000	0.0000	5087.5778	41.2888	0.0000
-0.0000	-0.0000	0.0000	41.2888	3972.5701	-0.0000
-61.3601	23.8853	90.1952	0.0000	-0.0000	4597.8293

[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].