SACADA Database Code: 324

Topology: 4^{12}T1

# of independent nodes (IN): 12
Transitivity: [(12)(18)(16)(10)]
Space Group: Pmc21
Pearson: oP24
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}T1 (SACADA #324)		3.412		0.759	389.6	441.0	82.8	SACADA[1]
S-S'2A2	15.4							doi: 10.1103/PhysRevLett.108.135501

Elasticity tensor (kBar)[1]

10933.4157	980.9181	1106.6714	0.0000	-0.0000	0.0000
980.9181	11056.3256	314.6591	-0.0000	-0.0000	0.0000
1106.6714	314.6591	8565.8107	-0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	5103.8870	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	3654.0585	0.0000
0.0000	0.0000	0.0000	-0.0000	0.0000	4128.8338

[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].