**SACADA Database Code: 329**

Topology: $4^{12}$T4

# of independent nodes (IN): 12
Transitivity: [(12)(20)(19)(11)]
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 |
|---|---|---|---|---|---|---|---|---|
| $4^{12}$T4 (SACADA #329) | | 3.483 | | 0.628 | 417.5 | 484.7 | 91.5 | SACADA[1] |
| S-S1Z4 | 3.8 | | | | | | | doi: 10.1103/PhysRevLett.108.135501 |
| S-S1Z4 | | | | | | | | doi: 10.1103/PhysRevB.93.085201 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 10293.6943 | 1171.4171 | 1244.0237 | -0.0000 | 0.0000 | 107.0001 |
| 1171.4171 | 11198.6510 | 295.0383 | -0.0000 | 0.0000 | -98.1182 |
| 1244.0237 | 295.0383 | 10669.7422 | -0.0000 | -0.0000 | -65.8786 |
| -0.0000 | -0.0000 | -0.0000 | 5289.1245 | -127.0984 | -0.0000 |
| 0.0000 | 0.0000 | -0.0000 | -127.0984 | 4262.5507 | -0.0000 |
| 107.0001 | -98.1182 | -65.8786 | -0.0000 | -0.0000 | 4962.4982 |

[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].