**SACADA Database Code: 291**

Topology: $4^8$T16

# of independent nodes (IN): 8
Transitivity: [8(14)(12)7]
Space Group: C2/m
Pearson: mS32
Coordination Number (CN): 4

Year: 2015

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $4^8$T16 (SACADA #291) | | 3.456 | | 0.675 | 429.1 | 490.0 | 92.2 | SACADA[1] |
| mS32 | 0-20 | 3.418 | 4.5 | | 415 | | 90.8 | doi: 10.1039/c4cp04569f |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 10985.9067 | 383.6956 | 889.7178 | -0.0000 | 0.0000 | 313.2885 |
| 383.6956 | 11582.6240 | 1002.7427 | 0.0000 | -0.0000 | -202.0731 |
| 889.7178 | 1002.7427 | 11527.7848 | 0.0000 | -0.0000 | -140.5836 |
| -0.0000 | 0.0000 | 0.0000 | 4148.5658 | -245.8980 | 0.0000 |
| 0.0000 | -0.0000 | -0.0000 | -245.8980 | 5335.7938 | -0.0000 |
| 313.2885 | -202.0731 | -140.5836 | 0.0000 | -0.0000 | 4542.7086 |

[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].