**SACADA Database Code: 398**

Topology: $4^8$T27

# of independent nodes (IN): 8
Transitivity: [8(18)(12)3]
Space Group: P-1
Pearson: aP16
Coordination Number (CN): 4

Year: 2017

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $4^8$T27 (SACADA #398) | | 3.436 | | 0.822 | 404.8 | 451.4 | 84.5 | SACADA[1] |
| G89 | | | | | | | | doi: 10.1002/cphc.201700151 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 9018.1786 | 1546.9846 | 1330.8041 | 95.3331 | -153.1299 | 206.1679 |
| 1546.9846 | 9168.8454 | 999.0095 | 57.7113 | 33.4169 | -2.9544 |
| 1330.8041 | 999.0095 | 10532.2212 | -130.7629 | 112.4608 | 27.0400 |
| 95.3331 | 57.7113 | -130.7629 | 4764.4389 | 374.1681 | -23.4632 |
| -153.1299 | 33.4169 | 112.4608 | 374.1681 | 4661.9281 | 181.5344 |
| 206.1679 | -2.9544 | 27.0400 | -23.4632 | 181.5344 | 4978.6185 |

[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].