**SACADA Database Code: 531**

Topology: $4^2$T21-CA

# of independent nodes (IN): 2
Transitivity: [2565]
Space Group: P3221
Pearson: hP12
Coordination Number (CN): 4

Year: 2021

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $4^2$T21-CA (SACADA #531) | | 3.560 | | 1.518 | 388.6 | 374.1 | 65.6 | SACADA[1] |
| $4^2$T21-CA | | | | | | | | doi: 10.1038/s41524-021-00491-y |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 8270.3401 | 2185.9692 | 856.3912 | -0.3648 | -6.9006 | 230.8435 |
| 2185.9692 | 8297.4780 | 832.9271 | -1.2135 | 0.8625 | -243.7191 |
| 856.3912 | 832.9271 | 10702.2780 | 14.2999 | 11.4775 | 9.0209 |
| -0.3648 | -1.2135 | 14.2999 | 3055.8922 | -239.6187 | -2.1013 |
| -6.9006 | 0.8625 | 11.4775 | -239.6187 | 4080.0097 | -2.4270 |
| 230.8435 | -243.7191 | 9.0209 | -2.1013 | -2.4270 | 4062.9921 |

[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].