**SACADA Database Code: 415**

Topology: $4^3$T177

# of independent nodes (IN): 3
Transitivity: [3641]
Space Group: C2
Pearson: mS10
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 |
|---|---|---|---|---|---|---|---|---|
| $4^3$T177 (SACADA #415) | | 3.313 | | 1.532 | 320.6 | 339.5 | 62.5 | SACADA[1] |
| G113 | | | | | | | | doi: 10.1002/cphc.201700151 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 6456.1674 | 1947.8971 | 594.2333 | 0.0000 | 0.0000 | -636.4425 |
| 1947.8971 | 6888.2620 | 953.1214 | -0.0000 | 0.0000 | -177.0784 |
| 594.2333 | 953.1214 | 8582.4262 | 0.0000 | 0.0000 | -305.0292 |
| 0.0000 | -0.0000 | -0.0000 | 3551.0961 | -249.9389 | -0.0000 |
| 0.0000 | -0.0000 | -0.0000 | -249.9389 | 3961.7986 | -0.0000 |
| -636.4425 | -177.0784 | -305.0292 | -0.0000 | -0.0000 | 3620.0525 |

[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].