**SACADA Database Code: 179**

Topology: NSI

# of independent nodes (IN): 3
Transitivity: [3652]
Space Group: C2/m
Pearson: mS12
Coordination Number (CN): 4

Year: 2013

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| NSI (SACADA #179) | | 3.293 | | 0.782 | 397.9 | 420.8 | 77.5 | SACADA[1] |
| 6B | | | | | | | | doi: 10.1103/PhysRevB.88.014102 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 11680.5352 | 586.4322 | 874.3964 | 0.0000 | -0.0000 | -395.3766 |
| 586.4322 | 10817.2330 | 765.6018 | -0.0000 | 0.0000 | -235.5830 |
| 874.3964 | 765.6018 | 9024.1428 | -0.0000 | 0.0000 | -448.2600 |
| 0.0000 | -0.0000 | -0.0000 | 4726.8223 | -665.8222 | 0.0000 |
| -0.0000 | 0.0000 | 0.0000 | -665.8222 | 3815.6372 | -0.0000 |
| -395.3766 | -235.5830 | -448.2600 | 0.0000 | -0.0000 | 3113.8070 |

[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].