**SACADA Database Code: 615**

Topology: bay

# of independent nodes (IN): 2
Transitivity: [2455]
Space Group: P6/mmm
Pearson: hP16
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 |
|---|---|---|---|---|---|---|---|---|
| bay (SACADA #615) | | 3.222 | | 0.443 | 366.8 | 290.0 | 40.1 | SACADA[1] |
| bay | | | | | | | | doi: 10.1038/s41524-021-00491-y |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 10017.5928 | 1426.4114 | 859.1033 | -0.0000 | -0.0000 | -0.0000 |
| 1426.4114 | 10017.5928 | 859.1033 | -0.0000 | 0.0000 | 0.0000 |
| 859.1033 | 859.1033 | 7197.0398 | -0.0000 | 0.0000 | 0.0000 |
| -0.0000 | -0.0000 | -0.0000 | 4295.5907 | -0.0000 | 0.0000 |
| -0.0000 | -0.0000 | 0.0000 | -0.0000 | 1737.1967 | -0.0000 |
| -0.0000 | 0.0000 | -0.0000 | -0.0000 | -0.0000 | 1737.1964 |

[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].