**SACADA Database Code: 209**

Topology: SiC12

# of independent nodes (IN): 4
Transitivity: [4554]
Space Group: R-3m
Pearson: hR24
Coordination Number (CN): 4

Year: 2011

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| SiC12 (SACADA #209) | | 3.546 | | 0.575 | 449.9 | 530.5 | 100.4 | SACADA[1] |
| 12R | 15 | 3.53 | 4.50 | | 474.6 | | | doi: 10.1103/PhysRevB.84.012102 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 11983.7423 | 1065.0289 | 400.0638 | -1.6092 | -262.7970 | 1.5756 |
| 1065.0289 | 11979.7050 | 401.9454 | 0.4313 | 262.4829 | 0.1784 |
| 400.0638 | 401.9454 | 12792.6447 | -1.5202 | 0.1948 | 1.0472 |
| -1.6092 | 0.4313 | -1.5202 | 5451.9761 | -1.0336 | -262.9026 |
| -262.7970 | 262.4829 | 0.1948 | -1.0336 | 4795.0346 | -0.6545 |
| 1.5756 | 0.1784 | 1.0472 | -262.9026 | -0.6545 | 4796.0489 |

[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].