**SACADA Database Code: 620**

Topology: deh2

# of independent nodes (IN): 3
Transitivity: [3786]
Space Group: Cmcm
Pearson: oS32
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 |
|---|---|---|---|---|---|---|---|---|
| deh2 (SACADA #620) | | 3.350 | | 0.259 | 405.5 | 416.1 | 75.7 | SACADA[1] |
| deh2 | | | | | | | | doi: 10.1038/s41524-021-00491-y |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 9078.5567 | 948.3904 | 997.3315 | -0.0000 | 0.0000 | 0.0000 |
| 948.3904 | 11084.2857 | 1104.0398 | -0.0000 | 0.0000 | 0.0000 |
| 997.3315 | 1104.0398 | 10363.0568 | -0.0000 | 0.0000 | -0.0000 |
| -0.0000 | -0.0000 | -0.0000 | 3900.2884 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 | 0.0000 | 0.0000 | 4844.3583 | -0.0000 |
| 0.0000 | 0.0000 | -0.0000 | 0.0000 | -0.0000 | 3177.2886 |

[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].