

## SACADA Database Code: 6

Topology: [pcu](#) 

# of independent nodes (IN): 1

Transitivity: [1111]







Space Group: Pm-3m

Pearson: cP1

Coordination Number (CN): 6

Year: 1987

## Data

Name	Pressure, GPa	Density, g/cm <sup>3</sup>	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcu (SACADA #6)				HPP				SACADA <sup>1</sup>
simple cubic								<a href="#">link</a> 
SC1	>2700		Metal					<a href="#">link</a> 
SC4								doi: <a href="https://doi.org/10.1063/1.123068">10.1063/1.123068</a> 
sc								doi: <a href="https://doi.org/10.1103/PhysRevB.59.733">10.1103/PhysRevB.59.733</a> 
SC4								doi: <a href="https://doi.org/10.1007/978-94-010-1013-9_1">10.1007/978-94-010-1013-9_1</a> 
SC1								doi: <a href="https://doi.org/10.1007/s11224-016-0782-1">10.1007/s11224-016-0782-1</a> 

<sup>1</sup> 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  $\Gamma$ -centered k-points mesh with a reciprocal-space resolution of  $2\pi \times 0.025 \text{ \AA}^{-1}$  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  $\text{\AA}^{-1}$  for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio  $\nu$  — 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].