SACADA Database Code: 185

Topology: csi

# of independent nodes (IN): 3
Transitivity: [3763]
Space Group: Im-3
Pearson: cI120
Coordination Number (CN): 4

Year: 1991

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
csi (SACADA #185)		2.655		1.129	301.3	282.9	48.6	SACADA[1]
csi								doi: 10.1038/352674a0

Elasticity tensor (kBar)[1]

7032.7757	1002.5820	1002.5820	-0.0000	-0.0000	0.0000
1002.5820	7032.7757	1002.5820	-0.0000	-0.0000	-0.0000
1002.5820	1002.5820	7032.7757	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	2711.3490	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	2711.3490	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	2711.3490

[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].