SACADA Database Code: 617

Topology: cjh36

# of independent nodes (IN): 2
Transitivity: [2696]
Space Group: P42/mmc
Pearson: tP24
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
cjh36 (SACADA #617)		3.149		0.582	349.9	322.6	54.6	SACADA[1]
cjh36								doi: 10.1038/s41524-021-00491-y

Elasticity tensor (kBar)[1]

9576.2361	720.6316	551.0177	0.0000	0.0000	0.0000
720.6316	9576.2361	551.0177	-0.0000	-0.0000	-0.0000
551.0177	551.0177	8731.6879	-0.0000	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	2631.3998	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	2646.2928	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	2646.2928

[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].