SACADA Database Code: 108

Topology: clh

# of independent nodes (IN): 2
Transitivity: [2332]
Space Group: P42/mmc
Pearson: tP8
Coordination Number (CN): 3

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
clh (SACADA #108)		2.900		0.982	345.7	127.8	18.8	SACADA[1]
GT-8		2.956			348.5	130.4		doi: 10.1039/c5cp01621e
H-1								doi: 10.1103/PhysRevLett.115.026403

Elasticity tensor (kBar)[1]

6924.2172	950.6828	1086.7765	-0.0000	0.0000	-0.0000
950.6828	6924.2172	1086.7765	-0.0000	-0.0000	0.0000
1086.7765	1086.7765	12006.8078	-0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	309.9884	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	637.7835	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	637.7799

[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].