SACADA Database Code: 112

Topology: cfc (Allotrope with "sp" atoms)

# of independent nodes (IN): 2
Transitivity: [2333]
Space Group: P63/mmc
Pearson: hP12
Coordination Number (CN): 2, 4 (1:2)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cfc (SACADA #112)		3.011		1.331	320.2	152.1	20.3	SACADA[1]
4HYD		3.1	Metal		313.8	165.4	59.3	doi: 10.1016/j.diamond.2014.04.005

Elasticity tensor (kBar)[1]

6491.9956	645.8243	656.0115	0.0000	0.0000	-0.0000
645.8243	6491.9956	656.0115	0.0000	-0.0000	0.0000
656.0115	656.0115	13471.1028	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	2923.0856	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	317.6856	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	317.6856

[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].