SACADA Database Code: 111

Topology: cfc

# of independent nodes (IN): 2
Transitivity: [2333]
Space Group: P63/mmc
Pearson: hP8
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cfc (SACADA #111)		3.547		0.573	451.4	532.0	100.7	SACADA[1]
cfc								doi: 10.1524/zkri.2013.1620
4H-diamond		3.6			453.4	548.9	98.1	doi: 10.1016/j.diamond.2014.04.005

Elasticity tensor (kBar)[1]

11991.5779	1092.0260	410.5812	-0.0000	-0.0000	-0.0000
1092.0260	11991.5779	410.5812	-0.0000	0.0000	0.0000
410.5812	410.5812	12814.5389	-0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	5449.7760	-0.0000	0.0000
0.0000	0.0000	0.0000	-0.0000	4819.1693	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	4819.1693

[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].