SACADA Database Code: 85

Topology: kfi

# of independent nodes (IN): 1
Transitivity: [1453]
Space Group: Im-3m
Pearson: cI96
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
kfi (SACADA #85)		2.426		0.851	255.1	166.6	18.9	SACADA[1]
CA8								doi: 10.1134/s1063776111060173
CA8								link

Elasticity tensor (kBar)[1]

5672.2519	990.0231	994.6088	13.1842	-7.6882	-1.7732
990.0231	5666.2550	995.1057	0.5737	12.4424	-5.2159
994.6088	995.1057	5663.1635	-5.3874	-0.2053	8.3086
13.1842	0.5737	-5.3874	1326.2739	-0.7792	1.0191
-7.6882	12.4424	-0.2053	-0.7792	1324.3293	1.1951
-1.7732	-5.2159	8.3086	1.0191	1.1951	1324.0564

[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].