SACADA Database Code: 167

Topology: kgn

# of independent nodes (IN): 3
Transitivity: [3532]
Space Group: P432
Pearson: cP56
Coordination Number (CN): 3

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
kgn (SACADA #167)		1.806		0.495	191.3	83.9	11.6	SACADA[1]
kgn								doi: 10.1007/s11224-016-0782-1

Elasticity tensor (kBar)[1]

2717.4144	1511.3565	1511.3565	0.0000	-0.0000	0.0000
1511.3565	2717.4144	1511.3565	0.0000	0.0000	0.0000
1511.3565	1511.3565	2717.4144	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	1046.6283	0.0000	-0.0000
-0.0000	0.0000	-0.0000	0.0000	1046.6283	-0.0000
0.0000	0.0000	-0.0000	-0.0000	-0.0000	1046.6283

[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].