SACADA Database Code: 181

Topology: cas

# of independent nodes (IN): 3
Transitivity: [3653]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 4

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cas (SACADA #181)		3.270		0.245	392.5	408.0	74.6	SACADA[1]
C_{CAS}		3.27	3.18		407.0		89.2	doi: 10.1063/1.4965721

Elasticity tensor (kBar)[1]

10762.3634	521.8363	540.1177	0.0000	-0.0000	0.0000
521.8363	11630.6809	693.0568	0.0000	-0.0000	-0.0000
540.1177	693.0568	9529.0384	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	4568.1583	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	2674.6272	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	3709.6940

[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].