SACADA Database Code: 375

Topology: jbw

# of independent nodes (IN): 2
Transitivity: [2442]
Space Group: Pmma
Pearson: oP6
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
jbw (SACADA #375)		3.226		0.932	368.1	354.9	62.3	SACADA[1]
G51								doi: 10.1002/cphc.201700151
D-carbon	63.7	3.20	4.33		369		86.58	doi: 10.1063/1.5037380

Elasticity tensor (kBar)[1]

7293.3153	499.9487	2381.5199	-0.0000	0.0000	0.0269
499.9487	10286.5018	617.5529	-0.0000	0.0000	0.0020
2381.5199	617.5529	8655.8603	0.0000	-0.0000	0.0293
-0.0000	-0.0000	0.0000	4072.4063	0.0135	-0.0000
0.0000	0.0000	-0.0000	0.0135	3636.2418	0.0000
0.0269	0.0020	0.0293	-0.0000	0.0000	2851.4379

[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].