SACADA Database Code: 215

Topology: 3^3,4T96

# of independent nodes (IN): 4
Transitivity: [4664]
Space Group: Cmmm
Pearson: oS24
Coordination Number (CN): 3, 4 (2:1)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^3,4T96 (SACADA #215)		2.503		0.563	269.5	107.3	15.5	SACADA[1]
C_{24}-D		2.55	1.58					doi: 10.1016/j.carbon.2016.08.015

Elasticity tensor (kBar)[1]

6510.9829	231.9891	912.1974	-0.0000	0.0000	0.0000
231.9891	6372.1473	649.6695	-0.0000	-0.0000	-0.0000
912.1974	649.6695	8030.9017	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	165.1933	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	966.1050	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	581.5043

[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].