SACADA Database Code: 155

Topology: 3^2,4T96

# of independent nodes (IN): 3
Transitivity: [3431]
Space Group: Imma
Pearson: oI20
Coordination Number (CN): 3, 4 (4:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T96 (SACADA #155)		1.954		0.679	214.0	113.9	14.2	SACADA[1]
ZGM-20		1.93	1.06					doi: 10.1002/adfm.201301077

Elasticity tensor (kBar)[1]

8905.5026	773.3893	577.0618	0.6811	0.1079	0.2000
773.3893	2824.2652	2313.7096	1.0416	-1.9174	0.4126
577.0618	2313.7096	2217.3720	-0.4942	3.6445	0.1749
0.6811	1.0416	-0.4942	2203.9883	3.4241	0.0275
0.1079	-1.9174	3.6445	3.4241	1913.8776	1.8868
0.2000	0.4126	0.1749	0.0275	1.8868	1852.0983

[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].