SACADA Database Code: 512

Topology: 4^3T91

# of independent nodes (IN): 3
Transitivity: [3542]
Space Group: Pnma
Pearson: oP12
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
4^3T91 (SACADA #512)		3.308		0.872	384.0	389.6	70.4	SACADA[1]
G227								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9889.4818	635.3095	1040.4970	-0.0000	0.0000	0.0000
635.3095	10484.0575	560.9070	0.0000	-0.0000	-0.0000
1040.4970	560.9070	9722.8219	-0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	3917.2181	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	3840.0182	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	2785.8236

[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].