SACADA Database Code: 339

Topology: 4^{16}T5

# of independent nodes (IN): 14
Transitivity: [(16)(21)(20)(16)]
Space Group: Imma
Pearson: oI88
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
4^{16}T5 (SACADA #339)		3.512		0.600	423.9	497.0	94.0	SACADA[1]
10(II)								doi: 10.1103/PhysRevB.93.085201

Elasticity tensor (kBar)[1]

11292.4202	280.0535	1223.7998	-0.0000	-0.0000	0.0000
280.0535	10990.7383	1263.2365	-0.0000	0.0000	0.0000
1223.7998	1263.2365	10330.3090	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	4388.6316	-0.0000	0.0000
-0.0000	0.0000	-0.0000	-0.0000	5227.9765	-0.0000
0.0000	0.0000	0.0000	-0.0000	-0.0000	5387.1492

[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].