SACADA Database Code: 421

Topology: 4^{16}T10

# of independent nodes (IN): 16
Transitivity: [(16)(32)(29)(13)]
Space Group: P1
Pearson: aP16
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^{16}T10 (SACADA #421)		3.394		0.909	394.1	427.6	79.4	SACADA[1]
G121								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8715.6893	1304.3491	1487.5243	-21.4335	195.1787	-18.5497
1304.3491	9974.6686	681.7215	110.4096	-531.7291	-29.4509
1487.5243	681.7215	9867.4241	7.5345	-117.6119	-63.8182
-21.4335	110.4096	7.5345	4607.8430	-9.0316	-55.9854
195.1787	-531.7291	-117.6119	-9.0316	4164.0385	31.5274
-18.5497	-29.4509	-63.8182	-55.9854	31.5274	4351.7828

[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].