SACADA Database Code: 436

Topology: 4^{16}T12

# of independent nodes (IN): 16
Transitivity: [(16)(32)(21)5]
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}T12 (SACADA #436)		3.419		0.917	391.5	441.0	82.7	SACADA[1]
G136								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8737.0837	1181.0556	1476.9980	209.0321	-83.4567	90.9679
1181.0556	9936.4704	782.0170	69.2221	60.3356	72.8175
1476.9980	782.0170	9701.8090	-33.9567	345.3587	38.9785
209.0321	69.2221	-33.9567	4656.2728	126.9469	-15.0283
-83.4567	60.3356	345.3587	126.9469	4325.3113	48.9786
90.9679	72.8175	38.9785	-15.0283	48.9786	4852.9165

[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].