SACADA Database Code: 453

Topology: 4^{16}T13

# of independent nodes (IN): 16
Transitivity: [(16)(32)(19)3]
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}T13 (SACADA #453)		3.284		1.052	362.9	362.9	65.1	SACADA[1]
G160								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10356.5502	936.7837	711.2902	-35.8439	94.9046	-89.1683
936.7837	7917.7071	1177.8045	193.3284	73.0614	-462.5958
711.2902	1177.8045	8868.9163	44.0826	-544.7892	190.9488
-35.8439	193.3284	44.0826	3204.3872	-42.6381	118.5910
94.9046	73.0614	-544.7892	-42.6381	3334.7943	187.7942
-89.1683	-462.5958	190.9488	118.5910	187.7942	3689.4707

[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].