SACADA Database Code: 459

Topology: 4^{16}T17

# of independent nodes (IN): 16
Transitivity: [(16)(32)(25)9]
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}T17 (SACADA #459)		3.395		0.992	378.9	418.1	78.1	SACADA[1]
G166								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8856.6381	1276.5820	1350.3682	68.9906	11.5325	25.0537
1276.5820	8672.5500	1002.0238	72.3438	-187.1840	-320.0335
1350.3682	1002.0238	9347.6129	-10.8146	-178.3842	248.6603
68.9906	72.3438	-10.8146	4611.2333	-72.6881	102.1873
11.5325	-187.1840	-178.3842	-72.6881	4079.6350	-66.6622
25.0537	-320.0335	248.6603	102.1873	-66.6622	4542.8150

[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].