SACADA Database Code: 477

Topology: 4^{12}T6

# of independent nodes (IN): 12
Transitivity: [(12)(24)(15)3]
Space Group: P1
Pearson: aP12
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^{12}T6 (SACADA #477)		3.325		1.140	372.0	385.1	70.3	SACADA[1]
G185								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8234.7988	1315.4386	1212.3931	-193.7530	-75.3809	-113.8313
1315.4386	8671.8511	1489.5738	42.8903	241.1349	-104.3564
1212.3931	1489.5738	8610.7947	-16.4927	513.1497	-348.5449
-193.7530	42.8903	-16.4927	3729.0119	4.0074	244.9224
-75.3809	241.1349	513.1497	4.0074	4132.5804	22.0375
-113.8313	-104.3564	-348.5449	244.9224	22.0375	4331.1689

[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].