SACADA Database Code: 458

Topology: 4^{16}T16

# of independent nodes (IN): 16
Transitivity: [(16)(24)(21)(13)]
Space Group: Cm
Pearson: mS32
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}T16 (SACADA #458)		3.419		0.777	396.4	445.1	83.5	SACADA[1]
G165								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

10294.8884	935.9002	1089.7701	0.0000	-0.0000	-190.0935
935.9002	10924.3138	471.2930	0.0000	-0.0000	182.4971
1089.7701	471.2930	9515.5795	-0.0000	0.0000	-358.1963
0.0000	0.0000	-0.0000	5096.5260	138.0230	0.0000
-0.0000	-0.0000	0.0000	138.0230	3915.5827	-0.0000
-190.0935	182.4971	-358.1963	0.0000	-0.0000	3972.6380

[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].