SACADA Database Code: 392

Topology: 4^{16}T8

# of independent nodes (IN): 16
Transitivity: [(16)(32)(32)(16)]
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}T8 (SACADA #392)		3.529		0.754	421.9	496.0	93.8	SACADA[1]
G81								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

11888.7658	836.8972	462.0930	5.1581	-125.3377	25.8133
836.8972	11059.6842	546.3994	4.3971	106.5149	73.7046
462.0930	546.3994	11349.9693	-3.0550	12.0927	-90.6464
5.1581	4.3971	-3.0550	5165.7186	4.2557	-126.9109
-125.3377	106.5149	12.0927	4.2557	4257.9429	5.2215
25.8133	73.7046	-90.6464	-126.9109	5.2215	4681.4402

[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].