SACADA Database Code: 418

Topology: 4^{16}T9

# of independent nodes (IN): 16
Transitivity: [(16)(32)(23)7]
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}T9 (SACADA #418)		3.373		0.932	388.5	415.7	76.9	SACADA[1]
G118								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8568.6584	1410.1410	1448.0929	-191.5358	191.4486	-107.4094
1410.1410	9383.9378	904.6387	-56.8463	-483.7495	-160.7792
1448.0929	904.6387	9566.4387	150.1639	-478.1481	-20.8326
-191.5358	-56.8463	150.1639	4478.2604	-57.3602	-79.3247
191.4486	-483.7495	-478.1481	-57.3602	4044.2037	7.8444
-107.4094	-160.7792	-20.8326	-79.3247	7.8444	4465.5778

[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].