SACADA Database Code: 454

Topology: 4^{16}T14

# of independent nodes (IN): 16
Transitivity: [(16)(32)(19)3]
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}T14 (SACADA #454)		3.384		0.974	387.2	416.4	77.1	SACADA[1]
G161								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8868.8137	1532.5348	1200.8755	-111.1661	259.4560	-186.8678
1532.5348	8346.2265	1222.4556	-186.6543	-646.6809	-20.4081
1200.8755	1222.4556	9904.7937	-215.8278	-692.9793	-67.6695
-111.1661	-186.6543	-215.8278	4289.7290	24.0199	-122.4143
259.4560	-646.6809	-692.9793	24.0199	4429.9299	-69.5229
-186.8678	-20.4081	-67.6695	-122.4143	-69.5229	4558.8712

[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].